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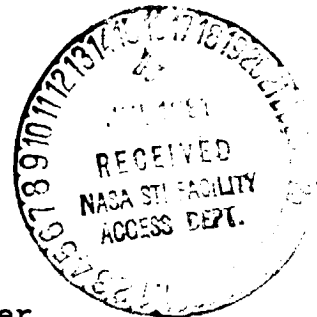
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ADDITION TO THE LEWIS CHEMICAL EQUILIBRIUM
PROGRAM TO ALLOW COMPUTATION FROM
COAL COMPOSITION DATA

DECEMBER, 1980

Prepared for:

NASA/George C. Marshall Space Flight Center
Huntsville Computer Complex



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Computer Sciences Corporation
Engineering Systems Department

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(Organization(s) that prepared this report:)

COMPUTER SCIENCES CORPORATION

ADDITION TO THE LEWIS CHEMICAL EQUILIBRIUM
PROGRAM TO ALLOW COMPUTATION FROM
COAL COMPOSITION DATA

DECEMBER, 1980

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APPENDIX A

--"Application of Lewis Chemical Equilibrium
Computer Program to Coal Gasification,"

by David Seymour A-1/A-10

APPENDIX B

--Source Listing of Program Elements with
Modifications.

B-1/B-120

APPENDIX C

--Source Listing of Program Elements Without
Modifications.

C-1/C-85

1.0 INTRODUCTION

This document reports changes made to the Lewis Chemical Equilibrium Program in order to adapt it for use by the Coal Gasification Project. The program was developed by the Lewis Research Center for analysis of the chemical equilibrium combustion in rocket engines. It can be applied directly to the entrained flow coal gasification process. The particular problem addressed is the reduction of the coal data into a form suitable to the program, since the manual process is involved and error prone. A similar problem in relating the normal output of the program to parameters meaningful to the coal gasification process was also addressed.

The revisions included in this writeup act as buffers on both sides of the Lewis Chemical Equilibrium Program to allow direct processing of raw coal gasification data and the production of data meaningful in coal gasification terms.

This document includes a Program Task Description of the capabilities created by the revisions of the original program. A list is given for the program elements which have been altered. Also included are two sample problems and a printout of the original program with and without the modifications for processing of coal gasification data.

The work was performed for the Engineering Systems Branch (AH33) of the Computer Services Office under contract NAS8-31640. The sponsoring organization was the Coal Gasification Task Team (PF15).

1.1 References

This program is self-contained and requires no other documents for its use and execution. Included for clarification are a memo by David Seymour, "Application of Lewis Chemical Equilibrium Computer Program to Coal Gasification" in Appendix A (Reference 2). If further revisions of this program become necessary, consult the "Computer Program for Calculation of Complex Chemical Equilibrium Compositions, Rocket Performance, Incident and Reflected Shock, and Chapman - Jouget Detonation" by Gordon and McBride, NASA SP-273 (Appendix B, Reference 1).

2.0 PROGRAM TASK DESCRIPTION

The Lewis Chemical Equilibrium Program was revised to include the following capabilities:

1. Accept data in the form of coal and other fuel element compositions and create reactant data compatible with the original program.
2. Store and edit the coal composition data.
3. Increase the number of elements within a compound from four to five.
4. Increase the number of reactants in the system from 15 to 25.
5. Provide a means of removing certain species from consideration during coal calculations.
6. Provide for coal data only, that input temperatures be in °F and that printout of pressure, temperature, enthalpy and entropy be in English units.
7. Provide, for coal data only, an additional section of output listing.
8. Allow the use of a new pseudo element, inert carbon.
9. Provide a store and edit feature for namelist list.
10. Provide that types of input data, as represented by various menuitems, be enterable in any order.
11. Simplify loading the program onto the terminal.
12. Provide a simple means of creating a copy of the system tape with the data from the previous run.

The program which provided the base for the revisions was "Computer Program for Calculation of Complex Chemical Equilibrium Compositions, Rocket Performance, Incident and Reflected Shock, and Chapman-Jouget Detonation" by Gordon and McBride, NASA SP-273. This program had been previously revised to provide interactive input and output via the Marshall Interactive Planning System (MIPS).

A complete listing of the source code is appended so that the changes indicated in the Revisions section may be followed.

3.0 REVISIONS OF LEWIS CHEMICAL EQUILIBRIUM PROGRAM

The current revision is discussed in relation to the changes required in various subroutines and how they relate to the new capabilities. Also discussed are the new inputs and outputs required or generated by the revision. Finally, a complete sample case, for coal data, is presented.

3.1 Storage Element A (Map overlay source code)

A new segment COALCV was added to handle the conversion of coal data to reactant data. Note that this segment is the longest and may at some future time have to be split into more segments.

3.2 Storage Element BLOCK1 (Miscellaneous data - Block data form)

The entry for atomic weight and valence of Deuterium was replaced with the atomic weight and valence of the pseudo element, inert carbon. The element symbol is IC and the weight and valence are those of regular carbon. The inert carbon element is used in the simulation of coal gasifier systems which have an unreacted carbon recycle stream.

3.3 Storage Element BOOT (Bootstrap control section)

The control statements serve to assign, copy and catalog the five files necessary to run the program. The catalog is included to insure that additional runs made on the same day do not have to reload the tape.

Note that BOOT is part of the first file on the system tape for the program. The following control statements are necessary to load the complete system:

```
@ASG,T PUR,U9S,XXXXX
@COPY,G PUR.TPF$.
@ADD TPF$.BOOT
```

The first part of Sample 1 shows the complete loading process.

File LEWIS contains all the subroutines and map elements. File 4 contains the thermodynamic data. Files 8, 10, and 12 contain dummy reactant data, namelist data and coal data, respectively.

3.4 Storage Element CHECK (Subroutine CHECK)

No changes.

3.5 Storage Element COALCV (Subroutine COALCV)

The subroutine COALCV is a new subroutine designed to do the major processing of converting coal composition data to reactant data.

The appended memo "Application of the Lewis Chemical Equilibrium Computer Program to Coal Gasification" by David C. Seymour (A-1) discusses the detailed calculations to be made based on the input data.

The subroutine assumes the existence of a previous set of coal data, stored in file 12. A set of coal reactant data immediately follows the coal data on file 12. This data is in the same form as the reactant data written by subroutine RREAD for data which is entered in the normal fashion. A dummy set of coal data is provided as part of the system tape. The user is queried as to whether he wants a printout of the previous data set. A response of YES produces a listing of the original coal data in the form shown in Sample 2. Regardless of whether a printout of the past data is requested, the past data is always read except for the conditions of first pass and no request for past data.

Table 1 explains the variables used by COALCV to store the coal data and the record groupings of the data. Table 2 explains the various possible measured or empirical values of higher heating value.

After printing the existing data, the user is prompted as to whether he wishes to modify the data, add to the data or continue with the same data. For the continue option, the subroutine exits. For the modify flag, a further prompt is given requesting the data group numbers of the data to be changed. See the last line of Sample 1. Each data group has associated with it a flag which indicates whether that type of data is to be processed. For the modify option, the flags of only those groups requested are turned on. For the add option, all flags are turned on.

Each data group flag is queried. If the flag is on, appropriate prompts are issued and the resulting information as entered by the user is stored in the appropriate variable. Two of the data groups, ash and other fuels, have additional special processing. For those data groups, two paths are possible. If the modify option was chosen, then it is possible to modify, delete or add individual lines to the existing material, via a series of prompts and responses. If the modify option was not chosen, the prompts and responses insert a completely new set of data.

Note that for ash composition, four of the common compounds are prompted for individually. If the weight of any of these is returned as 0 (or blank), that compound is eliminated. Note also that for other fuels, a search is made to determine which fuel number corresponds to water so that the proper water to coal ratio may be computed.

When all the required data groups have been entered, then the calculations outlined in the included paper are done, except for the section "Use and Interpretation of CEC Results". That section is done in another subroutine.

The coal data is saved on file 12 followed by the computed reactant data. The coal data is in the form shown in Table 1. The reactant data is in the same format as for the original program, except that the first record contains the coal to fuel ratio (CF) in addition to the number of reactants (NREAC). The subroutine then returns to the calling routine.

TABLE 1
COALCV VARIABLES

Record 1

NREAC	Number of reactants
CF	Coal to fuel ratio
HHVV	Higher heating value of coal Btu/lb
WCR	Water to coal ratio
PER	Fraction carbon conversion

Record 2

CTEMP	Coal temperature ($^{\circ}$ F)
OTEMP	Oxidizer Temperature ($^{\circ}$ F)

Record 3

PROX(3)	Proximate Analysis volatiles, fixed carbon, ash
COAL(5,2)	Coal composition in form element and number in order C, H, N, O, S.
PER	As above in record 2
IE	Pointer to higher heating value table
HH(8)	Measured and empirical higher heating value table. See table 2 for possible values.

Record 4

NCOAL	Number of other coal elements, other than C, H, N, O, S.
NASH	Number of ash compounds
NFUEL	Number of fuel compounds other than coal.
NOXID	Number of oxidizer compounds.

Record 5 *

CCOMP(12,5)	Other coal components in the form, weight, percent, state, and compound.
ACOMP(11,8)	Ash components in the form, weight percent and compound.
OFUEL(13,8)	Other fuel components in the form, weight, percent, temperature, state and compound.
OXID(11,5)	Oxidizer components in the form, weight percent and compound.

* Compound in this section indicates that a chemical compound is broken down into its component atoms and number of atoms. That is:
 $\text{CaCO}_3 = \text{Ca } 1.0 \text{ C } 1.0 \text{ O } 3.0$

TABLE 2

Possible Higher Heating Values

1	Measured Data
2	Dulong 1 $145.44(\%C) + 620.28(\%H - 1/8(\%O)) + 40.5(\%S)$
3	Dulong 2 $146.0(\%C) + 620.0(\%H - 1/8(\%O)) + 40.5(\%S)$
4	CPP2 $144.9(\%C) + 610.0(\%H - 1/8(\%O)) + 55.5(\%S)$
5	Grummel and Davis $\left[\frac{654.3(\%H)}{100. - \%Ash} + 424.62 \right] \left[\frac{\%C}{3} + \%H - \frac{\%O}{8} + \frac{\%S}{8} \right]$
6	Coal Conversion System Technical Data Base (CCSTDB) $146.58(\%C) + 568.78(\%H) + 29.4(\%S)$ $- 6.58(\%Ash) - 51.53(\%O + \%N)$
7	Maximum of 2 through 6
8	Minimum of 2 through 6

3.6 Storage Element CPHS (Subroutine CPHS)

Changes were made in the COMMON area MISC to accommodate 25 instead of 15 reactants. The variables changed were LLMT, B0, BOP, DATA, NAME (first dimension), ANUM (first dimension) PECWT, ENTH, FAZ, RTEMP, DENS, and RMW. In addition, the dimension of NAME (second dimension) and ANUM (second dimension) were changed to accommodate 5 elements within a compound rather than 4. Note that the last column of the array is used to store a flag indicating whether or not the enthalpy of the reactant is to be calculated.

3.7 Storage Element DETON (Subroutine DETON)

Same changes as for CPHS.

3.8 Storage Element EQLBRM (Subroutine EQLBRM)

Same changes as for CPHS.

Also increased temporary storage NROW to 25 from 15.

Added a temperature condition to the error message which states that "100 iterations did not satisfy the convergence requirement".

3.9 Storage Element FROZEN (Subroutine FROZEN)

Same changes as for CPHS.

3.10 Storage Element GAMEFF (Subroutine GAMEFF)

No changes.

3.11 Storage Element GAUSS (Subroutine GAUSS)

No changes.

3.12 Storage Element HCALC (Subroutine HCALC)

Same changes as for CPHS.

In addition the temporary storage area NUM was redimensioned 25 x 6. All references to NAM (N,5) or NAME (N,5) were changed to (N,6). All array processing of ANUM was increased by 1.

3.13 Storage Element LTCPHS (Subroutine LTCPHS)

No changes.

3.14 Storage Element MAIN (Subroutine MAIN - system driver)

Same changes as for CPHS in the data area. Also the addition of COMMON area CFUEL and the addition of a data area (NOMTS) which represent those species which can be eliminated from consideration when working with coal data. See Table 3 for a summary of the species. The upper limit of 150 possible species is often exceeded when using coal data. The optional omission species can be used to remove some of the least likely possibilities.

In the body of the subroutine the value of CF is initialized to -1.0. If CF remains as -1.0, then the coal data section was never entered since that section will produce a positive value of CF. The CF flag is used in other subroutines to initiate action required by the presence of coal data.

All the entries in namelist, INPT2, are initialized.

The menu of possible choices was expanded by addition of Item 7, 'start program calculation' and Item 8, 'insert or edit coal data.' The wording of Items 1 to 6 were reworked to make them consistent.

A request for Item 8 produces a call to subroutine COALCV and processing returns to the menu list. For menu Item 3, the call is made to subroutine RREAD rather than to subroutine REACT. This is to make the data entry independent of order. The decision on logical flag CALCH was moved to menu Item 7. In the move, references to NAME (N,5) were replaced with (N,6).

Menu Items 4 and 5 were corrected to properly store the species name being placed in the omit and insert lists.

Menu Item 6, concerning namelist, had an edit feature added. A dummy namelist is stored by the system on File 10. The user is queried as to whether he wishes to see the previous namelist. A response of YES prints the previous list and then the user is asked whether he wishes to change the namelist. The program either stops for new namelist data or returns to the menu list. A response of NO in the print namelist question, totally initializes the namelist and then stops to input new items. Return is to the menu list.

TABLE 3

Optional Omission Species

AL(S)	SI(S)
AL(L)	SI(L)
AL CL2	SICL
ALN(S)	SICL2
ALN	SICL3
C	SICL4
C3	SIH
C4	SIH4
C5	SIN
H2O(S)	SI2
O3	SI2O
SI	SI2N
SIC	SI3
SIC2	

Menu Item 7 was added to separate Item 6 from the actual start of the program so that Menu Items 1-6 and 8 can be input in any order. The new section moves the printout of the final namelist from Menu Item 6, the determination of logical CALCH from Menu Item 3 and the initialization of RHOP, VOL and NT from the original initialization area. In addition, this section requests the omission of the special coal data omit candidates.

Some special processing of Menu Item 7 is required by the exclusion of coal data. If the fraction of carbon conversion (PER) is less than 1, the special inert carbon element must be placed in the insert list. If the logical flag ERATIO is false and flag CF is positive then all MIX values must be multiplied by CF. MIX supposedly represents oxidizer to fuel ratio. For coal data, it is more convenient to input oxidizer to fuel ratio. The internally calculated coal to fuel ratio (CF) is then used to adjust to the proper O/F ratio. Also all namelist temperatures read in °F when coal data is being used, are adjusted to °K.

3.15 Storage Element MATRIX (Subroutine MATRIX)

Same changes as for CPHS.

3.16 Storage Element OUT1 (Subroutine OUT1 entries OUT2, OUT3, OUT4)

Same changes as for CPHS.

In addition, for coal data only, an additional line is printed at the end of the OUT1 printout. The line identifies oxidizer/coal ratio, water/coal ratio and fraction carbon conversion.

In the OUT2 section, for coal data only, pressures are printed in lbs per square inches, temperatures in °F, enthalpy in Btu/lb, entropy in Btu/(lb °F), and density in lb./cu.ft. The program pauses at the end of OUT2 to produce hardcopy of the output.

In the OUT3 section, for coal data only, an extra header line is printed. It is exactly the same as the line printed by OUT1.

The OUT4 section is new and corresponds exactly to the section "Use and Interpolation of CEC Results."

Sample 3 shows the printout created by each section of OUT1.

3.17 Storage Element PROK (PDP Element PROK)

No changes.

3.18 Storage Element REACT (Subroutine REACT)

Same changes as for CPHS.

Addition of common area CFUEL. Dimension changes of temporary variables ANAME, V, LLMTS, SBOP changes to array processing to handle 25 instead of 15 reactants. Change array processing ANUM and NAME to handle extra element within reactant.

The call to subroutine RREAD was removed and placed in MAIN. REACT now creates the final reactant data arrays by adding reactants placed on the reactant file (4) by the normal reactant input and those coal data reactants which are stored on the coal data file (12). The subroutine uses a two pass system. The first pass reads the first record from the coal data file if CF is -1. This places necessary header data into the system. If any normal reactants exist, they are read into the appropriate data areas. When all the reactants are read, the coal data reactants are read and added to the appropriate data areas.

3.19 Storage Element RKTOUT (Subroutine RKTOUT)

Addition of COMMON area CFUEL.

A call to OUT4 if coal data is present.

3.20 Storage Element ROCKET (Subroutine ROCKET)

Same changes as in CPHS.

Added a prompt for namelist RKTINP.

3.21 Storage Element RREAD (Subroutine RREAD)

Temporary arrays NAME, ANUM, PECWT, MOLE, ENTH, FAZ, RTEMP, FOX, DENS were adjusted to handle 25 instead of 15 reactants. NAME and ANUM were also adjusted to handle an additional element within the reactant. Array processing of these arrays was adjusted accordingly. The COMMON area CFUEL was added.

The first record of the reactant file was amended to include the value of CF. The individual reactant lines were adjusted to isolate the code which indicates that the enthalpy should be calculated. Previously, it had been recorded as part of the NAME array.

In addition, the edit section was made two pass. In the first pass, the data which is added or edited, is placed on the reactant file. Data to be edited also comes from this file. On the second pass, if one is requested, it is taken from the coal reactant data portion of the coal data file. Updates and/or additions are made to this data and the changed data is returned to the coal data file behind the original coal data. Note that the reactant data from the two sources is not added together until subroutine REACT, which is part of the startup routine. The setting of flag FIRST was removed from subroutine RREAD.

3.22 Storage Element SAVE (Subroutine SAVE)

Same changes as for CPHS. Addition of COMMON area CFUEL.

Creation of an additional header line, for coal data only. The line contains oxidizer/coal ratio, water/coal ratio and fraction carbon conversion. This header occurs just before the summation of atoms in the system.. See Sample 2, labeled SAVE.

3.23 Storage Element SEARCH (Subroutine SEARCH)

Same changes as for CPHS. Added a specific number for number of species in system. Also added a pause at the end of the species printout to obtain a hardcopy.

3.24 Storage Element SHCK (Subroutine SHCK)

Same changes as for CPHS.

3.25 Storage Element TAPESAVE (Tape Save Control Section)

The control statements serve to assign a tape, called LEWISTAPE, and copy the five system files into the tape. The following statement is necessary to call the tapesave system:

@ADD LEWIS.TAPESAVE

3.26 Storage Element THERMP (Subroutine THERMP)

Same changes as for CPHS. Added COMMON area CFUEL.

Addition of a pause to create a hardcopy of the material prior to the output of THERMP.

For coal data only, a call to entry OUT4 of subroutine OUT1.

Also, a pause at the end of THERMP to create a hardcopy before the next data set is processed.

3.27 Storage Element VARFMT (Subroutine VARFMT)

No changes.

3.28 Thermodynamic Data (File 4)

Thermodynamic data for the pseudo element inert carbon was added to the data. The data was that for C(S) with the exception of the compound name and atom name.

4.0 SAMPLE PROBLEM 1

The following pages indicate the procedure to load the Lewis Chemical Equilibrium Program and input new coal data into the system.

The data set which is being illustrated is the same as in the attached memo (A-1).

PORT 28/48 SIGNON - HOST1(2ND) LP HOST2(2ND) LP
 RTYP00
 ENTER USERID/PASSWORD
 >SALOWDS ESD

SDC:TPV USERID/PASSWORD ENTRY
 INITIATE 1100 OPERATING SYSTEM LEU AX30028H0571(MS1)S
 SEUIGNB1M20812(1) COPIED ON 08/04/80 AT 14:23:18
 DATE 081880 TIME 094804
 >AS: T PUP U95.02130
 READY

>COPY: G PUP TPF8
 FURPUP 28R1M1 E36 S74711 08/18/80 00:44:26
 SEUIGNB1M20812(1) COPIED ON 08/04/80 AT 14:23:18
 105 BLOCKS COPIED
 EOF ENCOUNTERED ON INPUT TAPE
 >COPY: TPF8 BOOT
 READY
 READY
 READY
 READY
 READY
 READY
 READY
 READY
 READY

FURPUP 28R1M1 E36 S74711 08/18/80 00:44:26
 105 BLOCKS COPIED
 SEUIGNB1M20812(1) COPIED ON 08/04/80 AT 14:24:49
 17 BLOCKS COPIED
 EOF ENCOUNTERED ON INPUT TAPE
 SEUIGNB1M20812(1) COPIED ON 08/04/80 AT 14:25:17
 1 BLOCK COPIED
 EOF ENCOUNTERED ON INPUT TAPE
 SEUIGNB1M20812(1) COPIED ON 08/04/80 AT 14:25:30
 1 BLOCK COPIED
 EOF ENCOUNTERED ON INPUT TAPE
 SEUIGNB1M20812(1) COPIED ON 08/04/80 AT 14:26:49
 1 BLOCK COPIED
 EOF ENCOUNTERED ON INPUT TAPE
 READY

4-4
4-5

08125 L
READY
FACILITY WARNING 100000000000
FILE HAS BEEN PREVIOUSLY ASSIGNED (OR FREED)
READY
FURNISH 28R1M1 E36 574T11 08/21/00 08 11 07
1 ARE
12 BLOCKS COPIED
12 BLOCKS COPIED
64 BLOCKS COPIED

MIPS INITIALIZATION IS IN PROGRESS
 OFF-LINE MAINTENANCE PROCESSOR LAST RUN AT 08/18/80 09.17.37
 TOTAL SUP TIME . 2 17 MIN
 SELECT NEW PRINT FILE OPTION.
 1 - WRITE PRINT FILE ON PAPER
 2 - WRITE PRINT FILE ON FICHE
 MIPS
 A PRINT FILE HAS BEEN ESTABLISHED NAMED MPS1055551XPSFS
 INSERT COMMANDS (INSERT HELP FOR TUTORING)
 MIPS>XQT LEUIS B
 MIPS>SU ONE
 SAME COMPLETED
 MIPS>RN ONE
 MIPS>GO

TYPE YES FOR PRINT TO PRINT FILE
NIPS

LEWIS CHEMICAL EQUILIBRIUM PROGRAM

MAIN MENU

1 - INSERT THERMODYNAMICS DATA
2 - INSERT LOW TEMP EXTENSION THERMO DATA
3 - INSERT OR EDIT REACTANTS
4 - OMIT SPECIES FROM THERMO DATA
5 - INSERT CONDENSED SPECIES
6 - INSERT OR EDIT NAMELIST
7 - START PROGRAM CALCULATION
8 - INSERT OR EDIT COAL DATA
9 - RETURN - TERMINATE PROGRAM

019578

TYPE YES TO READ IN PREVIOUS COMPOSITION
NIPS:10

MIPS>

```
TYPE (OPTIONAL) LBS VOLATILES/100 LBS DRY COAL
MIPS> 54
TYPE LBS ASH/100 LBS DRY COAL
MIPS> 83
TYPE COAL TEMPERATURE IN DEG F
MIPS> 0
TYPE LBS/100 LBS DRY COAL FOR ELEMENTS
(
MIPS> 31
H
MIPS> 5
N
MIPS> 529
O
MIPS> 343
S
MIPS> 1
TYPE (OPTIONAL) OTHER COAL COMPONENTS
TYPE LBS/100 LBS DRY COAL STATE AND AND COMPONENT
COAL TEMPERATURE IS ASSUMED
EXAMPLE 0 13 1HG 2MCL 2
MIPS> 13 1HG 2MCL 2
MIPS>
TYPE LBS/100 LBS DRY ASH FOR COMPONENTS
STATE ASSUMED SOLID COAL TEMPERATURE ASSUMED
5102
MIPS> 68
FE2O3
MIPS> 68
AL2O3
MIPS> 23
FE32
MIPS>
CONTINUE WITH ASH COMPONENTS
LBS/100 LBS DRY ASH AND COMPONENT
EXAMPLE 0 25 2HT 1 1M0 2
MIPS>
TYPE CARBON CONVERSION FRACTION FOR EXAMPLE 0 89
MIPS> 945
MMU CALCULATION
0 - ENTER DATA
1 - DULONG 1 12414 484
2 - DULONG 2 12451 687
3 - CPER 12308 885
4 - GRUNDEL-DAVIS 12423 143
5 - CCSTDB 12182 720
6 - MAX OF ABOVE 12451 687
7 - MIN OF ABOVE 12182 720
MIPS> 0
ENTER MMU AS BTU/LB COAL
MIPS> 12141
TYPE OTHER FUEL COMPONENTS
TYPE LBS/LB COAL TEMPERATURE (DEG F) AND STATE AND COMPONENT
EXAMPLE 0 31 100 1HG 1M0 2 1M0 1
MIPS> 0 1 212 1HG 1M0 2 1M0 1
MIPS>
TYPE IN OXIDIZER TEMPERATURE DEG F
MIPS> 7
TYPE OXIDIZER COMPONENTS
TYPE LBS/100 LBS OXIDIZER AND COMPONENT
EXAMPLE 95 0 1M0 2
MIPS> 95 1M0 2
MIPS> 5 2M0 1
```


LEWIS CHEMICAL EQUILIBRIUM PROGRAM

MAIN MENU

1 - INSERT THERMODYNAMICS DATA
2 - INSERT LOW TEMP EXTENSION THERMO DATA
3 - INSERT OR EDIT REACTANTS
4 - OMIT SPECIES FROM THERMO DATA
5 - INSERT CONDENSED SPECIES
6 - INSERT OR EDIT NAMELIST
7 - START PROGRAM CALCULATION
8 - INSERT OR EDIT COAL DATA
9 - RETURN - TERMINATE PROGRAM
MPS%

TYPE YES FOR PRINT INPT2 NAMELIST
PIPS>C
BEGIN NAMELIST INPT2 INPUT
> INPT2 MIX. 9: P.15 END

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LEWIS CHEMICAL EQUILIBRIUM PROGRAM

MAIN MENU

```

1 - INSERT THERMODYNAMICS DATA
2 - INSERT LOW TEMP EXTENSION THERMO DATA
3 - INSERT OR EDIT REACTANTS
4 - OMIT SPECIES FROM THERMO DATA
5 - INSERT CONDENSED SPECIES
6 - INSERT OR EDIT NAMELIST
7 - START PROGRAM CALCULATION
8 - INSERT OR EDIT COAL DATA
RETURN - TERMINATE PROGRAM
MIPS>>

```

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(MIPS)

THERMODYNAMIC EQUILIBRIUM PROPERTIES AT ASSIGNED PRESSURES

CHEMICAL FORMULA									
	C	H	N	O	S	WT FRACTION	ENTHALPY CAL/MOL	STATE	TEMP DEG K
FUEL	49.7311	44.3187	1.0251	0	3.7243	73034	-222076	S	298.15
FUEL	1.0000					03366	000	S	298.15
FUEL	2.0000					00118	000	S	298.15
FUEL	1.0000	0	2.0000			07726	-217699	S	298.15
FUEL	1.0000	0	3.0000			03754	-197250	S	298.15
FUEL	2.0000	0	3.0000			02912	-408493	S	298.15
FUEL	2.0000	0	1.0000			00991	-57188	S	373.15
FUEL	2.0000					05000	000	G	298.15
OXIDANT	0	2.0000				05000	000	G	298.15
OXIDANT	0	1.0000						G	298.15

O/F. 8273 PERCENT FUEL. 54.7264 EQUIVALENCE RATIO. 2.1776 DENSITY. 0000
 OXIDIZER/COAL. 9100 WATER/COAL. 100 CARBON CONVERSION. 9450

THERMODYNAMIC PROPERTIES

PRESS PSIA 15.000
 TEMP DEG F 3447.10
 ENTH BTU/LB -930.13
 S BTU/(LB-R) 2.8403
 DENSITY L/FRA3 8.492-03
 M MOL WEIGHT 23.7175
 (DLU/DLP) T -1.0065
 (DLU/DLP) P 1.1430
 CP CAL/(G-K) 1.7021
 GAMMA (S) 1.1753
 SON VEL M/SEC 1191.73

READ/COPY - THIS INPUT WILL NOT BE INTERPRETED
 MIP5

OXIDIZER/COAL- 9100 WATER/COAL- 1000 CARBON CONVERSION- 9450

WILE FRACTIONS

AL02H	7 679-07
AL2O3.S1	3 501-03
AL	1 270-02
CO	5 495-01
CO2	4 342-04
CO2	4 072-02
CO2	2 344-05
CO2	1 022-06
CO2	2 785-06
FEIL	3 811-03
FEIL	1 876-03
FEIL2	0 580-07
FEIL2	2 159-05
FEIL2	5 450-05
FEIL2	2 188-03
FEIL2	4 036-04
FEIL2	2 311-01
FEIL2	8 658-02
FEIL2	4 854-03
FEIL2	3 436-02
FEIL2	8 163-07
FEIL2	6 083-03
FEIL2	7 293-07
FEIL2	1 079-04
FEIL2	4 359-04
FEIL2	1 895-03
FEIL2	8 704-04
FEIL2	5 018-04
FEIL2	2 552-03
FEIL2	1 095-03
FEIL2	1 364-02
FEIL2	3 464-06
FEIL2	1 323-24
FEIL2	12141 00
FEIL2	22 406
FEIL2	8376
FEIL2	29 01858
FEIL2	294 69
FEIL2	70435
FEIL2	28 5818
FEIL2	290 12
FEIL2	281 06
FEIL2	285 28
FEIL2	2 84

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MIPS)

5.0 SAMPLE PROBLEM 2

The following pages which could be a continuation of Sample 1, indicate the procedures to be used to edit existing coal data and/or existing namelist data.

The data set, after editing will still be the same as in the attached memo, but additional namelist options are illustrated.

TYPE YES FOR PRINT TO PRINT FILE
MIPS: NO

LEWIS CHEMICAL EQUILIBRIUM PROGRAM

MAIN MENU

1 - INSERT THERMODYNAMICS DATA
2 - INSERT LOW TEMP EXTENSION THERMO DATA
3 - INSERT OR EDIT REACTANTS
4 - QUIT SPECIES FROM THERMO DATA
5 - INSERT CONDENSED SPECIES
6 - INSERT OR EDIT NAMELIST
7 - START PROGRAM CALCULATION
8 - INSERT OR EDIT COAL DATA
9 - RETURN - TERMINATE PROGRAM

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TYPE YES TO READ IN PREVIOUS COMPOSITION
MIPS>ES

TYPE YES TO READ IN PREVIOUS COMPOSITION

MIPS> ES
1 - VOLATILE (OPTIONAL) AND ASH AS LBS/100 LBS DRY COAL
VOLATILE 37 5400
ASH 15 8300

2 - ANAL TEMPERATURE IN DEG F 77 00

3 - DRY COAL COMPOSITION AS LBS/100 LBS DRY COAL

C 67 3100
H 4 7570
N 1 5200
O 6 3430
S 4 1000

4 - OTHER COAL COMPONENTS AS LBS/100 LBS DRY COAL. STATE AND COMPOSITION

1300 C CL 2 0000 0000 0000

5 - ASH COMPOSITION AS LBS/100 LBS ASH AND COMPONENT

53 6800 SI 1 0000 0 2 0000 0000
26 0800 FE 2 0000 0 3 0000 0000
20 2300 AL 2 0000 0 3 0000 0000

6 - FRACTION CARBON CONVERSION 9450

7 - HEATING VALUE OF COAL BTU/LB 12141 000

8 - OTHER FUEL COMPONENTS AS LBS/LB COAL. TEMPERATURE IN DEG F. STATE AND COMPOSITION

1000 212 000 C H 2 0000 0 1 0000 0000

9 - OXIDIZER TEMPERATURE IN DEG F 77 00

10 - OXIDIZER COMPONENTS AS LBS/100 LBS OXIDIZER AND COMPONENT

95 0000 O 2 0000 0000 0000
5 0000 AR 1 0000 0000 0000

TYPE 1 OR 2 TO MODIFY OR REPLACE

RETURN TO CONTINUE

MIPS>1

TYPE GROUP NUMBERS OF DATA TO BE CHANGED IN ASCENDING ORDER FOR EXAMPLE 1 3 7 9

MIPS>2 5 6


```

TYPE COAL TEMPERATURE IN DEG F
MIPS>T
GROUP NUMBER S
1 53 6800 SI 1 0000 0 2 0000
2 26 0800 FE 2 0000 0 3 0000
3 20 2300 AL 2 0000 0 3 0000
TYPE 1-ALTER 2-DELETE 3-ADD. RETURN TO CONTINUE
MIPS>
TYPE LINE NUMBER
MIPS>1
LBS 100 LBS DRY ASH AND COMPONENT
MIPS>3 68 2451 1 140 2
1 53 6800 SI 1 0000 0 2 0000
2 26 0800 FE 2 0000 0 3 0000
3 20 2300 AL 2 0000 0 3 0000
TYPE 1-ALTER 2-DELETE 3-ADD. RETURN TO CONTINUE
MIPS>
TYPE CARBON CONVERSION FRACTION. FOR EXAMPLE. 0.89
MIPS>N 945

```

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INDEX	REACTANT(8)	REL WT/ MO MOLES	MOLE	ENTHALPY/ INT ENERGY	PHASE	TEMP.K	FUEL/ OXID	DENSITY
1	C 49 7311 H 44 3187 N 1 0251 0 3 7243 S 1 2008	730336	-222076	00001	S	298 150	F	00000
2	IC 1 0000	033655	00001	00001	S	298 150	F	00000
3	CL 2 0000	001182	00001	00001	G	298 150	F	00000
4	SI 1 0000	077258	00001	00001	S	298 150	F	00000
5	FE 2 0000	037535	00001	00001	S	298 150	F	00000
6	AL 2 0000	020116	00001	00001	S	298 150	F	00000
7	PM 2 0000	000000	00001	00001	G	373 150	F	00000
8	MO 2 0000	050000	00001	00001	G	298 150	O	00000
9	AR 1 0000	050000	00001	00001	G	298 150	O	00000

INDICATES ENTHALPY TO BE CALCULATED

TYPE 1, 2 OR 3 TO MODIFY, DELETE, OR ADD A REACTANT (RETURN TO CONTINUE)

MIPS) YES FOR SPECIAL OMITS FOR COAL DATA

MIPS) YES

LEWIS CHEMICAL EQUILIBRIUM PROGRAM

MAIN MENU

1 - INSERT THERMODYNAMICS DATA
2 - INSERT LOW TEMP EXTENSION THERMO DATA
3 - INSERT OR EDIT REACTANTS
4 - OMIT SPECIES FROM THERMO DATA
5 - INSERT CONDENSED SPECIES
6 - INSERT OR EDIT NAMELIST
7 - START PROGRAM CALCULATION
8 - INSERT OR EDIT COAL DATA
9 - RETURN - TERMINATE PROGRAM

WPS>>

TYPE YES FOR PRINT INPT2 NAMELIST

01MPT2
 DETN
 ERATIO
 FA
 FPCY
 HP
 IDERUG
 IONS
 MIX

5

0	0	0	0	0
0	2	4	6	8
0	2	4	6	8
0	2	4	6	8
0	2	4	6	8

0
OF
NISON
MCH

. . . .

L L T

150000E+02
000000E+00
000000E+00
000000E+00
000000E+00
000000E+00
000000E+00
000000E+00

PSIA	.
RKT	.
S0	.
SHOCK	.
S0	.
SP	.
SU	.
T	.

L. L. L.
 . . .
 TP 23-

000000E+00
000000E+00
000000E+00
000000E+00

```
SEND  
BEGIN NAMELIST INPT2 INPUT  
> $INPT2 WP= F . T=2500 . TP= T SEND
```


LEWIS CHEMICAL EQUILIBRIUM PROGRAM

MAIN MENU

1 - INSERT THERMODYNAMICS DATA
2 - INSERT LOW TEMP EXTENSION THERMO DATA
3 - INSERT OR EDIT REACTANTS
4 - OMIT SPECIES FROM THERMO DATA
5 - INSERT CONDENSED SPECIES
6 - INSERT OR EDIT NAMELIST
7 - START PROGRAM CALCULATION
8 - INSERT OR EDIT COAL DATA
9 - RETURN - TERMINATE PROGRAM
MIPS>

SPECIES BEING CONSIDERED IN THIS SYSTEM

J 12/65 AL	J 6/70 ALCL	J 6/70 ALCL3(L)	J 6/70 ALCL3
J 6/63 ALH	J 6/70 ALCL	J 12/67 ALCL3(L)	J 12/67 ALCL3
J 12/68 AL2H	J 6/70 AL2CL6	J 9/64 ALCL	J 12/68 AL2
J 6/72 AL203(L)	J 5/65 AL	J 6/72 AL20	J 12/68 AL203(S)
J 6/70 CL3	J 12/68 CCL4	J 3/61 CCL	J 12/68 CCL2
J 6/69 CH	J 3/61 CH4	J 12/67 CH	J 3/61 CH20
J 9/55 CO	J 12/65 COCL	J 6/69 CH	J 12/70 CH2
J 12/82 CO	J 6/51 CS2	J 6/61 COCL2	J 9/65 CO2
J 3/61 CH2	J 6/55 CS2	J 12/69 C2H6	J 3/67 C2H
J 9/66 CO2	J 6/68 C2H4	J 5/72 C2H6	J 3/61 C2H2
J 3/61 CLO2	J 6/65 C3O2	J 6/72 CLO	J 3/61 CLO
J 3/65 FE(S)	J 9/65 CLE	J 3/65 FE	J 3/65 FE(S)
J 12/70 FECL2(L)	J 3/65 FECL2	J 6/65 FECL3(S)	J 12/70 FECL2(S)
J 6/65 FO(S)	J 12/70 FECL2	J 6/65 FECL3(L)	J 6/65 FECL3
J 6/66 FECL3(S)	J 12/70 FECL4	J 6/65 FECL3(S)	J 12/66 FECL3
J 3/64 H2O	J 9/64 HCL	J 12/69 HCN	J 9/65 H
J 3/63 HNO	J 6/63 HNO2	J 6/63 HNO3	J 12/70 HNO
J 11/65 H2O(L)	J 6/63 H2O	J 12/69 H2O2	J 3/61 H2
J 3/61 N	J 12/70 HCO	J 12/71 H	J 3/61 IC(S)
J 6/63 NO	J 12/72 NOCL	J 9/64 M2	J 9/65 NH3
J 9/55 N2	J 12/65 N2H4	J 12/64 M2	J 12/64 M203
J 12/70 N3	J 6/62 O	J 12/64 M20	J 12/64 M205
J 12/65 S(L)	J 6/71 S	J 12/70 OH	J 12/65 S(S)
J 6/61 S02	J 6/71 S02CL2	J 6/67 SH	J 6/71 S0
J 6/67 S102(S)	J 6/71 S102(S)	J 9/65 S03	J 9/67 S10
J 12/71 S15	J 3/67 S12C	J 6/67 S102(S)	J 9/67 S102

READ/COPY - THIS INPUT WILL NOT BE INTERPRETED
(RIPS)

OF	827273	OXIDIZER/COAL	9100	WATER/COAL	1000	CARBON CONVERSION	9450					
		FUEL	OXIDANT	MIXTURE								
M	CAL/G	- 94422572+03	00000000	- 51674044+03								
KG-ATOMS/KG												
C		481+2209-01	00000000	26346483-01								
H		52995222-01	00000000	29002360-01								
N		99234840-03	00000000	54307624-03								
O		12785041-01	59377227-01	33879015-01								
S		11624379-02	00000000	63615839-03								
IC		28020050-02	00000000	15334356-02								
CL		33340215-04	00000000	18245889-04								
SI		12858276-02	00000000	70368676-03								
FE		47009607-03	00000000	25726651-03								
AL		57112435-03	00000000	312555561-03								
AR		00000000	12516271-02	56665704-03								
PT	C	ADD AL2O3(S)	M	O	S	IC	CL	SI	FE	AL	AR	
1	-9 188	-10 135	-15 662	-26 504	-14 718	-2 362	-31 193	-14 064	137	-13 333	-25 133	17 000
1	-9 171	-10 127	-15 660	-26 516	-14 728	-2 362	-30 929	-14 048	137	-30 310	-25 130	5 000
1	-9 151	-10 119	-15 659	-26 532	-14 739	-2 362	-30 060	-14 031	-4 764	-30 286	-25 127	5 000
1	-8 950	-10 094	-15 650	-26 702	-14 574	-2 362	-30 074	-24 839	-4 538	-30 032	-25 111	5 000
1	-10 979	-10 439	-15 651	-24 994	-14 115	-2 362	-29 706	-28 254	-6 814	-32 593	-25 112	5 000
1	-9 032	-10 102	-15 650	-26 627	-14 561	-2 362	-30 038	-24 989	-6 814	-30 144	-25 111	5 000

SAVE

EOLBRM

9450

CARBON CONVERSION-

1000

WATER/COAL-

9100

OXIDIZER/COAL-

MOLE FRACTIONS

AL2O3(S)	3 521-03
AR	1 227-02
CO	5 397-01
CO2	9 251-04
CS	5 301-02
CS2	8 364-06
FE(S)	3 615-06
FE	5 792-03
FECL2	2 150-06
FE2O3	6 799-07
H	2 680-06
HCL	4 014-05
H2	4 097-04
H2O	2 400-01
H2S	7 442-02
IC(S)	1 197-02
N2	3 455-02
OH	6 118-03
S	5 401-07
SH	4 332-06
SO	2 246-04
SO2	1 140-05
S2	1 319-05
SiO2(S)	5 828-04
	1 586-02
MMU COAL B/LB	12141 00
MIXTURE MW	22 533
MF OF CDG	85165
V SAT SCF/LB	28 26287
MMU SAT B/SCF	290 28
EFFICIENCY	69964
V DRY SCF/LB	28 82986
MMU DRY B/SCF	294 64
LHU SAT B/SCF	276 32
LHU DRY B/SCF	280 47
B PER MMBTU	2 86

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READ/CONV - THIS INPUT WILL NOT BE INTERPRETED
NIPS)

GENES CHEMICAL EQUILIBRIUM PROGRAM

MAIN MENU

- 1 - INSERT THERMODYNAMICS DATA
- 2 - INSERT LOW TEMP EXTENSION THERMO DATA
- 3 - INSERT OR EDIT REACTANTS
- 4 - OMIT SPECIES FROM THERMO DATA
- 5 - INSERT CONDENSED SPECIES
- 6 - INSERT OR EDIT NAMELIST
- 7 - START PROGRAM CALCULATION
- 8 - INSERT OR EDIT COAL DATA
- 9 - RETURN - TERMINATE PROGRAM

***** MIPS MODULE TERMINATED. SUP'S USED • 26 SECONDS *****

NORMAL EXIT CPU TIME 12388 TOTAL SUPS 27808 (MILLISECONDS)

***** COMPLETE *****

TOTAL SUP TIME * 2.80 MIN
 IS THE CURRENT PRINT FILE TO BE TRANSMITTED?
 MIPS:NO
 INSERT COMMANDS (INSERT HELP FOR TUTORING)
 MIPS:SP
 MIPS IS EXITING
 PRINT FILES WILL BE DELETED IF NOT TRANSMITTED
 IS THE CURRENT PRINT FILE TO BE TRANSMITTED?
 MIPS:NO
 NORMAL EXIT CPU TIME 20 TOTAL SUPS 7084 (MILLISECON
 DS:STOP MIPS
 @FIN

PUNID LEWIST ACCT 1HPD013K000 PROJECT SEVIGNBIN208
 LOAD BLANK TP6 N25LEWIS -1 LEWIST
 *** SAVE *** 24609 TP6 N25LEWIS
 SEVIGNBIN208XN25LEWIS 24609 082180
 STOP MIPS
 LEWIST FIN

TIME TOTAL 00 02 52 840 CBSUPS 047260104
 CPU 00 00 10 552 I/O 00 01 24 660
 CC/ER 00 01 17 627 WAIT 00 27 40 234
 IMAGES READ 116 PAGES 13
 START 10 39 03 AUG 18.1980 FIN 11 12 02 AUG 18.1980

 * THERE WILL BE A USERS MEETING ON 9/10/80 AT 09:00 A M IN THE HOSC *
 * CONFERENCE ROOM AT BLDG 4663. ALL USERS ARE URGED TO ATTEND. *

 DEMAND USERS PLEASE KEYIN @USER*RESPONSE.POLL PRIOR TO @FIN (THANK YOU)

 TERMINAL INACTIVE

APPENDIX A
APPLICATION OF LEWIS CHEMICAL EQUILIBRIUM
COMPUTER PROGRAM TO COAL GASIFICATION
BY
DAVID SEYMOUR

This copy of a NASA memo describes the calculations of input and output used in the sample problems for conversion to coal gasification data.

George C. Marshall Space Flight Center
Marshall Space Flight Center, Alabama
35812

Reply to Attn of PF15 E/0-118)

August 28, 1980

TO: PF15/John P. McCarty

FROM: PF15/David C. Seymour

SUBJECT: Application of the Lewis Chemical Equilibrium Computer Program to Coal Gasification

REF: (a) "Computer Program for Calculation of Complex Chemical Equilibrium Compositions, Rocket Performance, Incident and Reflected Shocks, and Chapman-Jouguet Detonations" NASA SP-273, Gordon and McBride

(b) "Fortran IV Computer Program for Calculation of Thermodynamic and Transport Properties of Complex Chemical Systems", NASA TN-D-7056, Svehla, McBride

In the early 1960's Lewis Research Center developed a chemical equilibrium combustion (CEC) computer program for rocket engine performance analysis (Ref. (a)). Because of the thorough documentation, flexibility, and comprehensive specie library, the program has become an aerospace industry standard.

The CEC program can be applied to entrained flow coal gasification without modification. The complete thermodynamic state can be described for either adiabatic combustion or specified temperature and pressure. The procedures used to apply the program to coal gasification are described here, together with a sample case. Because these procedures are somewhat tedious and error prone, a subroutine has been added to the CEC program which contains these procedures.

The CEC program requires the chemical formula, relative amount and enthalpy of each reactant in the system. For a typical entrained flow gasifier, the reactants include steam, oxygen (with nitrogen and argon impurities) and coal. Due to the complex composition of coal, the chemical formulae for the coal components are generally not supplied and must be determined from an elemental analysis.

Consider the ultimate analysis of the dry Kentucky #9 used by TVA for design criteria.

Coal Composition		Ash Composition	
Element	% Wt.	Compound	% Wt.
C	67.31	SiO_2	45.94
H	4.757	Al_2O_3	17.31
N	1.529	Fe_2O_3	22.29
O	6.343	CaO	5.486
S (Pyritic)	2.517	MgO	1.164
S (Non Pyritic)	1.583	SO_3	3.264
Cl	.131	Na_2O	.557
Ash	15.83	K_2O	2.336
	<u>100.00</u>	TiO_2	.742
		Other	.911
			<u>100.00</u>

The term ash used here refers to the residue obtained from complete oxidation of the coal with excess air during a proximate analysis of the coal.

The compounds existing in the coal are unknown. In particular, the composition of the ash is not the same as the composition of the minerals in the coal and thus the ash mass fraction in the coal indicated above is not the true mineral content of the coal. The sodium and potassium, for example, probably exist in the coal as chlorine salts or as part of the other inorganic compounds. Most of the iron in the coal exists as iron pyrite, FeS_2 .

The details of the compounds in the coal and ash are not required for an equilibrium combustion calculation. Only the relative amounts of the elements present must be known. The ash composition shown above is actually an elemental composition with fictitious oxide compounds assumed and is not a real ash composition. The actual ash composition is dependant on the amount of oxygen available during combustion, the combustion temperature, and the rate of cooling of the combustion products.

The ultimate analysis of coal shown above consists of direct measurement of the amount of elemental C, H, N, S, and Cl. The ash weight is then added and the oxygen content is taken to be the difference between 100 and this sum. Thus, if the only remaining element in the coal is oxygen, the oxygen content which is obtained plus the oxygen in the fictitious ash compounds represents the true total elemental oxygen in the coal. The fictitious ash compounds can be used directly to describe the relative amounts of the elements and corrections to the ash content or further assumptions about the coal composition are not required. The only exception is that the sulfur in the ash should not be included, since it is already accounted for in the elemental sulfur in the coal. However this correction is smaller than the accuracy of the data and is not included here.

Determination of CEC Reactant Data From Coal Composition

The elemental mass composition of the coal must be converted into a atom/ (mole reactant) form for input to the CEC. Since the program is limited to five elements per reactant, a reacting coal is arbitrarily defined to be composed of C, H, N, O and S. Other elements and compounds known to exist in the coal are treated as individual reactants.

Since some of the carbon in the coal may not actually be oxidized, a carbon conversion factor, f , is defined as the mass fraction of carbon which participates in the reaction. The remaining carbon is removed from the reacting coal and treated as an inert solid with carbon thermodynamic properties.

As an example of the procedure, the composition of the reacting coal for the previously described Kentucky #9 is, with $f = .945$

Coal Element	<u>lb Element</u> <u>100 lb coal</u>	<u>lb Element</u> <u>100 lb coal</u>	<u>lb Element</u> <u>100 lb reacting coal</u>
C	67.31	63.61	79.18
H	4.757	4.757	5.921
N	1.529	1.529	1.903
O	6.343	6.343	7.896
S	4.10	<u>4.10</u>	<u>5.103</u>
Cl	.131	80.337	100.00
Ash	<u>15.83</u>		
	100.00		

Converting to lb-atoms/(lb-mole reacting coal) gives

Element	<u>lb Element</u> <u>lb-atom</u>	<u>lb-atoms</u> <u>100 lb reacting coal</u>	<u>lb-atoms</u> <u>100 lb-mole reacting coal</u>
C	12.01	6.593	49.74
H	1.008	5.874	44.31
N	14.007	.136	1.03
O	16.00	.494	3.73
S	32.064	<u>.159</u>	<u>1.20</u>
		13.256	100.00

Then the chemical formula for the reacting coal is

C_{49.74} H_{44.31} N_{1.03} O_{3.73} S_{1.20}

and it's molecular weight per 100 lb-mole is

$$\frac{(100)}{13.256} \times 100 = 754.4 \text{ lb}/(100 \text{ lb-mole})$$

$$= 754.4 \text{ g}/(100 \text{ g-mole reacting coal})$$

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Relative Reactant Weights

In coal gasification it is convenient to use as independent variables the mass ratios water/coal (or steam/coal) and oxygen/coal. The CEC program, however, allows only one independent variable, oxidizer/fuel (O/F). The components of the system identified as oxidizers as opposed to fuels is completely arbitrary. The distinction between oxidizer and fuel is only important when running multiple O/F values within a single execution of the program.

The convention selected here is $\text{fuel} = \text{coal} + \text{H}_2\text{O} + (\text{other fuel compounds})$,

where $\text{coal} = \text{reacting coal} + \text{minerals} + \text{inert C} + (\text{other coal compounds})$.

Oxidizer = O_2 + (impurities in O_2 feed),

where the other fuel and coal compounds and the O_2 impurities must be included in the CEC thermodynamic data library.

Then

$$\frac{\text{coal}}{\text{fuel}} = \frac{1}{1 + \frac{\text{H}_2\text{O}}{\text{coal}} + \frac{(\text{other fuel compounds})}{\text{coal}}}$$

and the relative weight of reacting coal in the fuel, required for input to the CEC is

$$\frac{\text{reacting coal}}{\text{fuel}} = \frac{\text{coal}}{\text{fuel}} \frac{(\text{reacting coal})}{\text{coal}}$$

similarly, for the other components of the fuel,

$$\frac{\text{minerals}}{\text{fuel}} = \frac{\text{coal}}{\text{fuel}} \frac{(\text{minerals})}{\text{coal}}$$

$$\frac{\text{inert C}}{\text{fuel}} = \frac{\text{coal}}{\text{fuel}} (1-f) \frac{(\text{carbon})}{\text{coal}}$$

$$\frac{\text{H}_2\text{O}}{\text{fuel}} = \frac{\text{coal}}{\text{fuel}} \frac{(\text{H}_2\text{O})}{\text{coal}}$$

and for the oxidizer

$$\text{CEC O/F} = \frac{\text{coal}}{\text{fuel}} \frac{(\text{O}_2)}{\text{coal}}$$

where O_2/coal includes the impurities.

As an example, suppose an equilibrium calculation were to be run for Kentucky # 9 with $f = .945$, $H_2O/\text{coal} = .10$, and $O_2/\text{coal} = .91$, where the O_2 feed is 95% pure O_2 and 5% Ar by volume. Then the relative weights are

$$\frac{\text{coal}}{\text{fuel}} = \frac{1}{1 + .10} = .9091$$

$$\frac{\text{reacting coal}}{\text{fuel}} = .9091 (.8034) = .7304$$

$$\frac{\text{minerals}}{\text{fuel}} = .9091 (.1583) = .1439$$

$$\frac{\text{inert C}}{\text{fuel}} = .9091 (1 - .945) (.6731) = .0337$$

$$\frac{H_2O}{\text{fuel}} = .9091 (.10) = .0909$$

$$\frac{Cl_2}{\text{fuel}} = .9091 (.00131) = \frac{.0012}{1.000}$$

$$\frac{O_2}{\text{Oxidizer}} = .975$$

$$\frac{Ar}{\text{oxidizer}} = .025$$

$$CEC O/F = .9091 (.91) = .8273$$

The relative weights of the ash components are, considering only the largest three,

$$\frac{SiO_2}{\text{fuel}} = .1439 \frac{(.4594)}{.8554} = .0773$$

$$\frac{Al_2O_3}{\text{fuel}} = .1439 \frac{(.1731)}{.8554} = .0291$$

$$\frac{Fe_2O_3}{\text{fuel}} = .1439 \frac{(.2229)}{.8554} = \frac{.0375}{.1439}$$

where the remaining ash components have been arbitrarily spread equally between these three.

Determination of Coal Enthalpy from HHV

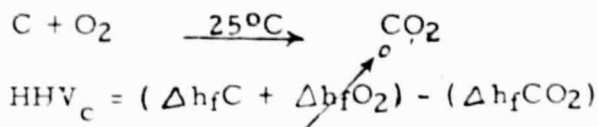
The CEC program requires an enthalpy for each reactant when calculating adiabatic flame conditions. Enthalpies are not required for calculating equilibrium conditions at specified temperature and pressure. The enthalpy of the reacting coal is the heat of formation at 25°C plus the enthalpy changes from 25°C to the coal temperature. HHV is the heat of combustion at 25°C, where the products of combustion are CO₂, H₂O (l), and SO₂. The HHV of coal is either measured in a calorimeter bomb test or obtained from an empirical formula based on the coal ultimate analysis.

The known HHV_{coal} can be broken down into the reacting components selected for CEC input as

$$\text{HHV}_{\text{coal}} = \text{HHV}_{\text{r. c.}} \left(\frac{\text{reacting coal}}{\text{coal}} \right) + \text{HHV}_{\text{c}} \left(\frac{\text{inert C}}{\text{coal}} \right)$$

The oxides in the ash all have an HHV of zero and do not have to be included here.

The HHV for carbon can be calculated from the heats of formation and the definition of HHV. For carbon,



Where Δh_{fC} = heat of formation of carbon, taken here to be amorphous carbon. $\Delta h_{\text{fC}} = 4680 \text{ BTU/lb-mole}$

$$\Delta h_{\text{fCO}_2} = -169293 \text{ BTU/lb-mole}$$

$$\text{HHV}_{\text{c}} = (4680 + 169293) \frac{1}{12.01} = 14486 \text{ BTU/lb carbon}$$

$$\text{Then the reacting coal HHV is} \quad \text{HHV}_{\text{rc}} = \frac{\text{HHV}_{\text{coal}} - 14486 \left(\frac{\text{inert C}}{\text{coal}} \right)}{\frac{\text{reacting coal}}{\text{coal}}}$$

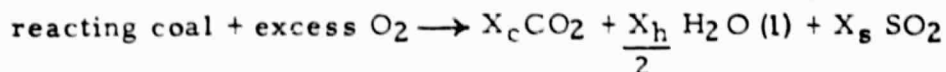
If, in the previous example, HHV_{coal} is given as 12141 BTU/lb coal then

$$\text{HHV}_{\text{rc}} = \frac{12141 - 14486 (.037)}{.8034}$$

$$= \frac{12141 - 536}{.8034}$$

$$= 14445 \text{ BTU/lb reacting coal}$$

The heat of formation of the reacting coal can be obtained from the definition of HHV. The reaction is



where X_c , X_h , X_s are the C, H, and S g-atoms per 100 g-moles of reacting coal.

The N and O in the coal are not included since their heat of formation is zero.

$$\text{Then } \text{HHV}_{rc} = \Delta h_{frc} - (X_c \Delta h_{f\text{CO}_2} + \frac{X_h}{2} \Delta h_{f\text{H}_2\text{O}} + X_s \Delta h_{f\text{SO}_2})$$

$$\text{where } \Delta h_{f\text{CO}_2} = -94051.8 \text{ cal/g-mole CO}_2$$

$$\Delta h_{f\text{H}_2\text{O (l)}} = -68317.4 \text{ cal/g-mole H}_2\text{O (l)}$$

$$\Delta h_{f\text{SO}_2} = -70960 \text{ cal/g-mole SO}_2$$

$$\Delta h_{frc} = \text{HHV}_{rc} - X_c (94051.8) - X_h (68317.4) - X_s (70960)$$

where the units of Δh_{frc} required by the CEC are cal/(100 g-mole reacting coal).

In the previous example,

$$\begin{aligned} \text{HHV}_{rc} &= (14445 \frac{\text{BTU}}{\text{lb reacting coal}}) (\frac{\text{cal/g}}{1.8 \text{ BTU/lb}}) (754.4 \frac{\text{g}}{100 \text{ g-mole}}) \\ &= 6.0540 \times 10^6 \text{ cal/(100 g-mole)} \end{aligned}$$

and

$$\begin{aligned} \Delta h_{frc} &= 6.0540 \times 10^6 - (49.74) (94051.8) - \frac{(44.31) (68317.4)}{2} \\ &\quad - (1.20) (70960) \\ &= 6.0540 \times 10^6 - 6.2769 \times 10^6 \\ &= -222890 \text{ cal/(100 g-mole reacting coal)} \end{aligned}$$

If the coal temperature were 25°C (77°F), then the coal enthalpy required by the CEC would be Δh_{frc} . For temperatures up to about 200°F, the reacting coal enthalpy can be estimated from the empirical equation.

$$h_{rc} - \Delta h_{frc} = .175 (T - 77) + .0029 W_v (T - 77) + .00025 (T - 60)^2 - .072$$

where T is the coal temperature in °F and W_v is the percent of volatiles in the dry, ash free coal given by proximate analysis.

If in the previous example, the proximate analysis were

Volatiles	37.54	37.54	44.60
Fixed Carbon	46.63	<u>46.63</u>	<u>55.40</u>
Ash	<u>15.83</u>	84.17	100.00
	100.00		

then $W_v = 44.60$ and if the coal temperature were 100°F

$$\begin{aligned}
 h_{RC} - \Delta h_{f_{RC}} &= .175 (23) + .0029 (44.6) (23) = .00025 (40)^2 - .072 \\
 &= 7.33 \frac{\text{BTU}}{\text{lb reacting coal}} \\
 &= (7.33) \frac{754.4}{1.8} = 3072 \text{ cal/(100 g-mole reacting coal)}
 \end{aligned}$$

and the enthalpy used in the CEC, h_{RC} , would be

$$h_{RC} = -222890 + 3072 = -219820 \text{ cal/(100 g-mole)}$$

The enthalpy of the remaining reactants will automatically be determined by the CEC program from a specified reactant temperature.

Use and Interpretation of CEC Results

The CEC output consists of the thermodynamic state variables and the specie mole fractions. For coal gasification several other parameters are of interest.

First, the molecular weight output by the program is an effective value meant for use in the ideal gas equation of state. This effective value is the mass of the system per mole of gas in the system and excludes the moles of solids and liquids. To convert to a true ratio of mass/mole for the system,

$$M_w = (\text{CEC } M_w) \left(1 - \sum_{\text{solid}} X_i \right) + \text{liquids}$$

where X_i = CEC mole fraction.

Historically, fuel gas properties are usually quoted on a standard cubic foot basis, with various conventions taken for standard conditions. The standard used here is a saturated gas at 60°F and 30 in. of mercury. With this standard 385.2 SCF will contain 1 lb-mole of dry fuel gas. If the standard were dry gas at 60°F and 30 in. of mercury, 379.5 SCF would contain 1 lb-mole of dry fuel gas.

The moles of dry product gas per total moles of reactants is taken to be

$$X_{DP} = X_{CO} + X_{H_2} + X_{CH_4} + X_{CO_2} + X_{N_2} + X_{Ar}$$

The volume of clean, dry gas produced per lb of coal is then

$$Y_{DP} = \frac{385.2 X_{DP}}{M_w} \frac{\text{Reactants}}{\text{coal}}, \text{ SCF/(lb coal)}$$

where the mass fraction $\frac{(\text{Reactants})}{\text{coal}}$ can be obtained as $\frac{(\text{fuel} + O_2)}{\text{coal coal}}$.

The higher heating value of the gas, in BTU/SCF, is obtained from the HHV of the constituents as

$$HHV = \frac{319.24 X_{H_2} + 316.06 X_{CO} + 994.4 X_{CH_4}}{X_{DP}}$$

The lower heating value, which takes water vapor rather than liquid water as the reference state, is given by

$$LHV = \frac{269.71 X_{H_2} + 316.06 X_{CO} + 895.3 X_{CH_4}}{X_{DP}}$$

Cold gas efficiency, which is the fraction of the coal chemical energy converted to a gas chemical energy, is

$$E = \frac{HHV Y_{DP}}{HHV_{\text{coal}}}$$

where HHV_{coal} is the higher heating value of dry coal and does not include any of the previously discussed corrections for carbon conversion.

The equilibrium thermochemical data provided by the program represent an idealized state and must be applied to actual gasifier operation with caution. The major non-equilibrium effect, unreacted carbon, had been accounted for in this application of the CEC program. However, as the gas/particle mixture is cooled within the gasifier, the chemical reaction rates will decrease and chemical equilibrium will no longer be maintained. A freeze point temperature can be defined as that temperature at which the equilibrium composition approximates the final non-equilibrium temperature. This freeze point temperature must be determined by a finite rate analysis or experimental data. When the freeze point temperature is known, the CEC program can be applied with a specified temperature and pressure to describe the final gas composition.

If transport property data is required, the CEC program described in Ref (B) can be used in lieu of Ref. (A).

David C. Seymour

David C. Seymour

Distribution:

PF15/Messrs. Rutland/Klan/Irby/Costes/Deaton/Garrett/Hyde/Johnston/
Kramer/Larsen/Lynn/Middleton/Stonemetz

PF15/Dr. Proffitt

PD31/Mr. Davies

PD11/Messrs. Howell/Rood/Kearns/Wells

PD21/Messrs. Peoples/Hall/Mundie/Sutherlin

PD33/Mr. Stafford

PD31/Messrs. Cole/Goss/Steincamp/Wheeler/Belcher

PP03/Mr. Hamaker

EF43/Messrs. Piner/Spear

APPENDIX B

SOURCE LISTING OF PROGRAM ELEMENTS
WITH MODIFICATIONS

This is a printout of the Lewis Chemical Equilibrium Program
with the modifications necessary for coal gasification data.

BRUN LEMIST, J, 101R50021, SEVIGNBIN208, 30,200

MSG,N REMOVE AT CARD READER 10-15-80 CLOCK NO 2709

MSG,T PUR,U95,15753

2COPY,B PUR.,T,F5.
FURPUR 26R1H1 E33 574T11 10/15/80 13:09:46
SEVIGNBIN208,LEWIS111 COPIED ON 09/18/80 AT 13:23:53
105 BLOCKS COPIED.
EOF ENCOUNTERED ON INPUT TAPE

2XOT,A SYS8MSFCS-LISTIT

2HDG,P A

2PRT,S A
FURPUR 26R1H1 E33 574T11 10/15/80 13:05:53

DATE 101500

A

SEVIGRIN208+TPF3(03).A
LIB LEWIS., MIPS+ILIB., SYS+MSFCs.

- 1 SEG DRIVER
- 2 IN LEWIS.BLOCK1
- 3 IN LEWIS.MAIN
- 4 SEG 00+IDRIVER)
- 5 IN LEWIS.COALCV
- 6 SEG 1+IDRIVER)
- 7 IN LEWIS.SEARCH
- 8 SEG 2+IDRIVER)
- 9 IN LEWIS.REACT
- 10 SEG 3+IDRIVER)
- 11 IN LEWIS.THERMP
- 12 SEG 4+IDRIVER)
- 13 IN LEWIS.DETON
- 14 SEG 5+IDRIVER)
- 15 IN LEWIS.SHCK
- 16 SEG 6+IDRIVER)
- 17 IN LEWIS.ROCKET
- 18

BLOCK1

ENDG.P

ORIGINAL PAGE IS
OF POOR QUALITY

FOR 5 BLOCK1,BLOCK1
MSA 23 -10/15/80-11:05:54 (11.)

BLOCK DATA

STORAGE USED: CODE(1) 000000; DATA(0) 000000; BLANK CODE(2) 000000

COMMON BLOCKS:

3 CONSTS 000006
888 HOLCON 000010
0005 MISC 001701
0006 OUP 000073

STORAGE ASSIGNMENT (BLOCK, TYPE, RELATIVE LOCATION, NAME)

0005	000640	AM	0005	000705	AM1	0005	001135	ANUM	0005	R	000004	ATAM	0005	R	000235	ATEM			
0003	R	000000	ATM	0005	000004	AT04	0005	000514	BO	0005	R	000545	RDP	0005	R	000706	CPRI		
0005	000634	CPSUM	0005	000654	DATA	0005	001560	DENS	0004	R	000000	END	0005	R	001700	ENLSAV			
0005	000000	CNN	0005	001676	ENNL	0005	001677	ENSAVE	0006	R	000005	F8	0006	R	000006	FC			
0006	R	000002	FA	0006	R	000003	FAP	0005	001445	FAZ	0006	R	000015	FG	0006	R	000017	FGE	
0006	R	000007	FCP	0006	R	000012	FCST	0006	R	000014	FCV	0006	R	000015	FG	0006	R	000017	FGE
0006	R	000020	FCV	0006	R	000021	FM	0006	R	000023	FI	0006	R	000025	FIV	0006	R	000027	FM
0004	R	000031	PMY	0006	R	000050	FM	0006	R	000052	FOUR	0005	R	000053	FP	0006	R	000053	FP
0006	R	000054	FS	0006	R	000056	FSV	0006	R	000057	FT	0006	R	000061	FTK	0006	R	000063	FV
0006	R	000067	FVEL	0006	R	000001	F13	0006	R	000000	F9X	0004	R	000001	GAS	0003	R	000001	GMEY
0005	000641	HPP	0005	000637	MSUB0	0004	I	000002	IE	0004	I	000003	IZERO	0004	I	000004	LANK		
0005	000643	LLMT	0004	I	000005	MOL	0005	000707	NAME	0005	000635	OF	0006	R	000047	JNE			
0004	R	000006	OX	0005	001644	OXF	0003	R	000002	PATM	0005	001363	PECMI	0005	R	000633	PP		
0003	R	000003	RRAP	0003	R	000004	RBR	0005	000644	RH	0005	001611	RHOP	0005	R	001612	RHW		
0005	001476	RTEMP	0003	R	000005	RVR	0005	000001	SUMH	0005	000003	SD	0005	R	000632	THIGH			
0006	R	000070	THREE	0005	001643	TLN	0005	000630	TLOW	0005	000627	TM	0005	R	000631	TMI0			
0005	000002	TT	0006	R	000071	TWO	0005	000646	VMIN	0005	000650	VPLS	0005	R	000652	WP			
0004	R	000007	ZERO	0006	R	000072	ZEROF												

B-14

00101	1*	C	BLOCK DATA	ATM000001	000000
00101	2*		COMMON /CONSTS/	/CONSTS/	000000
00102	3*		COMMON /HOLCON/	/HOLCON/	000000
00103	4*		COMMON /MISC/		000000
00104	5*		COMMON /MISC/		000000
00104	6*		COMMON /MISC/		000000
00104	7*		COMMON /MISC/		000000
00104	8*		COMMON /MISC/		000000
00104	9*		COMMON /MISC/		000000
00104	10*		COMMON /MISC/		000000
00104	11*		COMMON /MISC/		000000
00105	12*		COMMON /MISC/		000000
00105	13*		COMMON /MISC/		000000
00105	14*		COMMON /MISC/		000000
00105	15*		COMMON /MISC/		000000
00106	16*		COMMON /MISC/		000000
00107	17*		COMMON /MISC/		000000

```

C
00107 18* C ATOMIC SYMBOLS, WEIGHTS, AND VALENCES
00107 19* DATA ATAM/2HH, 1.00797, 1.0, 2HHE, 4.0026, 0.0, 2HLI, 6.939, 1.0, 2HBE,
00110 20* 1 9.0122, 2.0, 2HH, 10.811, 3.0, 2HC, 12.0115, 4.0, 2HN, 14.0067, 0.0,
00110 21* 2 2HC, 15.9998, 2.0, 2HF, 18.9988, 1.0, 0.2HNE, 20.163, 0.0, 2HNA, 22.9898
00110 22* 3 1.0, 2HMG, 24.312, 2.0, 2HAL, 26.9815, 3.0, 2HSH, 28.0864, 4.0, 2MP, 30.9738
00110 23* 4 5.0, 2HS, 32.064, 4.0, 2HCL, 35.453, 1.0, 2HAP, 39.988, 0.0, 2HK, 39.102,
00110 24* 5 1.0, 2HCA, 40.080, 2.0, 2HSC, 44.956, 3.0, 2HTI, 47.90, 0.0, 2HV, 50.942,
00110 25* 6 5.0, 2HCR, 51.996, 3.0, 2HNN, 54.9380, 2.0, 2HFE, 55.847, 3.0, 2HCO, 58.933,
00110 26* 7 2.0, 2HNI, 58.710, 2.0, 2HCU, 63.540, 2.0, 2HZN, 65.370, 2.0, 2HGA, 69.720,
00110 27* 8 3.0, 2HGE, 72.590, 4.0, 2HAS, 74.9216, 3.0, 2HSE, 78.960, 4.0, 2HHR, 79.909,
00110 28* 9 1.0, 2HHR, 83.80, 0.0, 2HRS, 85.47, 1.0, 2HSR, 87.620, 2.0, 2HY, 88.905,
00110 29* A 3.0, 2HTR, 91.220, 4.0, 2HNB, 92.906, 5.0, 2HMO, 95.946, 0.0, 2HTC, 99.0, 7.0,
00110 30* B 2HRU, 101.070, 3.0, 2HRH, 102.905, 3.0, 2HPO, 106.40, 2.0, 2HAG, 107.870,
00110 31* C 1.0, 2HCD, 112.40, 2.0, 2HIN, 114.820, 3.0, 2MSH, 118.690, 4.0, 2HSH,
00110 32* D 121.750, 3.0,
00110 33* DATA ATAM/2HTE, 127.60, 4.0, 2HI, 126.904, 1.0, 2HKE, 131.30, 0.0, 2HCS,
00110 34* 1 132.905, 1.0, 2HBA, 137.340, 2.0, 2HLA, 138.910, 3.0, 2HGE, 140.120, 3.0,
00112 35* 2 2HPR, 140.907, 3.0, 2HND, 144.240, 3.0, 2HPM, 145.0, 3.0, 2MSM, 150.350, 3.0,
00112 36* 3 2HEU, 151.960, 3.0, 2HGD, 157.250, 3.0, 2HTB, 158.924, 3.0, 2HGY, 162.50,
00112 37* 4 3.0, 2HMO, 164.930, 3.0, 2HER, 167.260, 3.0, 2HTM, 168.934, 3.0, 2HYB,
00112 38* 5 173.040, 3.0, 2HLU, 174.997, 3.0, 2HMF, 178.490, 4.0, 2HTA, 180.948, 5.0,
00112 39* 6 2HW, 183.650, 4.0, 2HRE, 186.20, 7.0, 2HOS, 190.20, 4.0, 2HIR, 192.20, 4.0,
00112 40* 7 2HPI, 193.090, 4.0, 2HAU, 196.97, 3.0, 2HMG, 200.590, 2.0, 2HIL, 204.370,
00112 41* 8 1.0, 2HPB, 207.190, 2.0, 2HBI, 208.980, 3.0, 2HPO, 210.0, 2.0, 2HAT, 210.0,
00112 42* 9 0.0, 2HQN, 222.0, 0.0, 2HFR, 223.0, 1.0, 2HRA, 226.0, 2.0, 2HAC, 227.0, 3.0,
00112 43* A 2HTH, 232.038, 4.0, 2HFA, 231.0, 5.0, 2HU, 238.030, 6.0, 2HNP, 237.0, 5.0,
00112 44* B 2HPU, 242.0, 4.0, 2HAM, 243.0, 3.0, 2HCH, 247.0, 3.0, 2HMK, 249.0, 1.0, 2HCF,
00112 45* C 251.0, 3.0, 2HES, 254.0, 0.0, 2HFM, 253.0, 0.0, 2HIC, 12.0115, 4.0,
00112 46* INFORMATION USED IN VARIABLE OUTPUT FORMAT
00112 47* C
00114 48* DATA F9X/3H9X, /, F13/2H13, /, FA/6HAE/AT, /, FB/6H /, FC/6HCF /,
00114 49* 1 FCV/6HCF VAC/AF6/12HRAHMA (S) /, FI/12HISP SECONDS /, /OUP/ /
00114 50* 2 FIV/12HIVAC SECONDS/ /, FM/12HM MOL WEIGHT/ /, FMT/6H1H, 2, /OUP/ /
00114 51* 3 6HA6, A2, 5SHF9, 1, 5SHF9, 1, 5SHF9, 1, 5SHF9, 1, 5SHF9, 1, 5SHF9, 1, /OUP/ /
00114 52* 4 5SHF9, 1, 5SHF9, 1, 5SHF9, 1, 5SHF9, 1, 5SHF9, 1, 5SHF9, 1, 5SHF9, 1, /OUP/ /
00114 53* 5 FN/12HMACH NUMBER /, FOUR/5HFE, 2, /, FP/6HPCP /, /OUP/ /
00114 54* 6 FT/12HIDLVL/DLP) T /, FV/12HOLV/DLP) P /, ONE/5HFE, 1, /, /OUP/ /
00114 55* 7 THREE/5HFE, 3, /, TWO/5HFE, 2, /, ZERO/5HFE, 0, /, FAP/12HPPRESS N/M**
00114 56* 82, /, FCP/12HCP CAL/IG1(K, 2H) /, FCST/12HCSTAR M/SEC /, FGE/6HIEFF) /,
00114 57* 9 FGV/6HGAS VE, /, FH/12HENTH CAL/G /, FS/12HS CAL/IG1(K) /, FSV/6HSON V
00114 58* AE, /, FTM/12HTEMP DEG. K /, FVEL/6HL M/SE, 2HC /
00114 59* DATA END/3HEND/6AS/1HG, /, IE/1HE, /, IZERO/2HQQ/ALANK/2H /, /MOL/1HM/
00153 60* 1 ,OX/1HO, /, ZERO/1HO, /, ATMN/101325.0, /, RVR/82.0554497/
00153 61* 3 ,GME/79.806650, /, PATM/14.6960060, /, RBR/1.9871650, /, RBR/8314.298360/
00172 62* END

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END OF COMPILATION: NO DIAGNOSTICS.

ADG,P BOOT

APRT,S BOOT

FURPUR 28R1H1 E33 574T11 10/15/80 13:05:56

ORIGINAL PAGE IS
OF POOR QUALITY

```

SEVIGMBIN208*IPFS(0)*BOOT
1  @CAT,P LEWIS F/64/TRM/128
2  @CAT,P A,F/64/TRM/1.
3  @CAT,P A,F/10/TRM/32
4  @CAT,P 10,F/10/TRM/32
5  @CAT,P 12,F/10/TRM/64
6  @AS,A LEWIS.
7  @AS6,A 4.
8  @AS6,A 8.
9  @AS6,A 10.
10 @AS6,A 12.
11 @COPY IPFS,LEWIS.
12 @COPY,G PUR,4.
13 @COPY,G PUR,8.
14 @COPY,G PUR,10.
15 @COPY,G PUR,12.
16 @FREE PUR.
    
```

@HOG,P CHECK

FOR,S CHECK,CHECK
HSA E3 -10,15,80-13:05:57 (2,)

SUBROUTINE CHECK ENTRY POINT 000056

STORAGE USED: CODE(1) 000065; DATA(1) 000013; BLANK COMMON(2) 000000

EXTERNAL REFERENCES (BLOCK, NAME)

0003 NERR3s

STORAGE ASSIGNMENT (BLOCK, TYPE, RELATIVE LOCATION, NAME)

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0000 000007 INJPS 0000 I 000003 JHIGH 0000 I 000004 JLOW

00101	1*		SUBROUTINE CHECK(NAME)	000000
00101	2*	C		000000
00101	3*	C		000000
00103	4*		BLANK FILL SPECIES SYMBOLS	000000
00107	5*		DATA IBLNK2/2H /, JHIGH/1H2/, ILOW/1HA/	000000
00114	6*		DATA JHIGH/0/, JLOW/0/, ICHAR1/0/, ICHAR2/0/	000000
00115	7*		FLO(10,6, ICHAR1)=FLO(10,6, NAME)	000000
00116	8*		FLO(10,6, ICHAR2)=FLO(10,6, NAME)	000001
00117	9*		FLO(10,6, JHIGH)=FLO(10,6, JHIGH)	000003
00120	10*		FLO(10,6, JLOW)=FLO(10,6, JLOW)	000005
00122	11*		IF (ICHAR1.LT. JLOW .OR. ICHAR1.GT. JHIGH) NAME=IBLNK2	000007
00122	12*	*	IF (ICHAR2.LT. JLOW .OR. ICHAR1.GT. JHIGH) FLO(10,6, NAME)=	000027
00124	13*		FLO(10,6, IBLNK2)	000047
00125	14*		RETURN	000064
			END	

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END OF COMPILATION: NO DIAGNOSTICS.

ENDG.P COALCY

FOR'S COALCV,COALCV
HSA E3 -10,15,80-13:05:9 (24,)

SUBROUTINE COALCV ENTRY POINT 003674

STOPA USED: CODE(1) 003713; DA,A(0) 003744; BLANK COMMON(2) 000000

COMMON BLOCKS:

0003 CFUEL 000000
0004 SPECES 017106
0005 INDX 000021
0006 CCC 000003

EXTERNAL REFERENCES (BLOCK, NAME)

0007 ROYES
0010 PAGIT
0011 CHRSTZ
0012 GOUT
0013 MNCODS
0014 RDATAI
0015 RDATAF
0016 MREWS
0017 MREWS
0020 NI02S
0021 NI03S
0022 NI01S
0023 MERR2S
0024 MREWS
0025 MREWS
0026 MERR3S

STORAGE ASSIGNMENT (BLOCK, TYPE, RELATIVE LOCATION, NAME)

0001	000030	10L	0000	002175	100F	0001	001444	10116	0001	001477	10256	0001	000460	104L
0001	001335	1040G	0000	002205	106F	0001	001743	10736	0000	002233	108F	0001	001764	11076
0001	000537	112L	0001	002063	1137G	0001	000554	114L	0001	002075	1147G	0001	000607	120L
0001	002213	1204G	0001	002213	1207G	0001	002246	1225G	0001	002316	1245G	0001	000617	126L
0001	002360	1270G	0001	002370	1273G	0001	000635	130L	0001	002454	1322G	0001	002531	1347G
0001	002541	1354G	0001	002553	1362G	0001	002565	1370G	0001	002576	1375G	0001	002607	1405G
0001	002653	1426G	0001	002733	1452G	0001	002734	1455G	0001	003021	1504G	0001	003034	1511G
0001	003035	1514G	0001	003213	1550G	0001	003214	1551G	0001	003253	1574G	0001	003263	1577G
0001	003322	1615G	0001	003407	1642G	0001	003422	1647G	0001	003423	1652G	0001	003544	1727G
0001	003564	1731G	0001	003571	1736G	0001	003571	1740G	0001	003576	1745G	0001	003576	1747G
0001	003603	1754G	0001	003603	1756G	0001	003620	1770G	0001	003624	1774G	0001	000011	205G
0001	000016	212G	0000	002404	2350F	0001	001102	2352L	0000	002410	2354F	0001	001137	2357L
0001	001143	2358L	0001	001177	2360L	0001	001250	2364L	0001	001254	2366L	0001	001257	2370L
0001	001263	2372L	0001	001315	2380L	0001	001352	2386L	0001	002053	2420L	0001	002116	2422L
0000	002547	2424F	0001	002112	2427L	0001	002152	2428L	0001	002216	2431L	0001	002222	2432L
0001	002225	2434L	0001	002231	2436L	0001	000126	256G	0001	000126	260G	0001	000133	265G
0001	000133	267G	0001	000140	274G	0001	000140	276G	0001	000637	300L	0001	000145	303G

COALCV

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0001 000145 1056 0001 000643 310L 0001 000660 312L 0001 000675 314L 0001 000677 316L
0001 000710 320L 0001 000718 322L 0001 000727 324L 0001 000740 326L 0001 000751 328L
0001 000762 330L 0001 000773 340L 0001 001013 342L 0001 000240 3436 0001 001017 343L
0001 001060 348L 0001 001063 350L 0001 001386 351L 0001 001366 352L 0001 001377 354L
0001 001421 358L 0001 001421 358L 0001 000273 3626 0001 001502 364L 0001 001520 366L
0001 001524 367L 0001 000302 3706 0001 001562 372L 0001 001565 380L 0001 001567 382L
0001 001600 390L 0001 002533 394F 0001 001773 400L 0001 002020 402L 0001 000335 4066
0001 000343 4136 0001 002031 420L 0001 002267 421L 0001 002301 422L 0001 002305 423L
0001 002347 428L 0001 002352 430L 0001 002405 434L 0001 002412 442L
0001 000434 4456 0001 002423 450L 0001 002437 452L 0001 000444 4546
0001 002504 460L 0001 002504 470L 0001 000160 50L 0001 000515 5006 0001 002706 504L
0001 000523 5056 0001 002767 520L 0001 000611 5336 0001 003070 540L 0001 000626 5436
0001 003276 552L 0001 003301 554L 0001 002020 56F 0001 003361 560L 0001 002024 58F
0001 003455 590L 0001 002032 60F 0001 002055 62F 0001 001030 6206 0001 001112 6546
0001 001122 6626 0001 003462 680L 0001 002100 70F 0001 001248 7176 0001 001245 7226
0001 001300 7406 0001 001323 7516 0001 001334 7546 0001 000316 80L 0001 002122 84F
0001 000357 90L 0001 002131 92F 0001 002143 94F 0001 011052 A 0001 003331 ACOMP
0001 000576 ANUM 0001 003461 ASH 0001 001776 ASHF 0001 001640 CC 0001 002744 CCOMP
0001 000000 CTEMP 0001 002732 COAL 0001 000000 COEF 0001 000001 CONV6 0001 001774 CSUM
0001 001780 CTEMP 0001 010624 DELM 0001 000002 DEMAND 0001 0001561 DEN5 0001 004312 EM
0001 001050 ENLM 0001 001447 ENH 0001 002676 FAZ 0001 001766 FES2 0001 002000 FES2C
0001 001531 FOX 0001 000000 GRAPH 0001 002001 HF1 0001 002003 HF2 0001 001734 HH
0001 001664 HHT 0001 001777 HNV 0001 000001 HHV 0001 000003 HP 0001 010376 HO
0001 001657 H2O 0001 001637 I 0001 003331 IACOMP 0001 003461 IASH 0001 001744 IC
0001 001645 ICC 0001 002744 ICCOMP 0001 002732 ICAL 0001 001625 ID 0001 000000 IDERUG
0001 001752 IE 0001 002676 IFAZ 0001 001652 IM20 0001 000015 IMAT 0001 003713 INJPS
0001 003040 IOFUEL 0001 001746 IOPT 0001 001760 IOU 0001 003242 IOXID 0001 002727 IPROX
0001 000016 IO1 0001 000005 ISV 0001 016266 IUSE 0001 001757 J 0001 001761 JJ
0001 001613 JOPT 0001 000001 JOU 0001 000014 KMAT 0001 001763 KOUT 0001 000012 L
0001 000000 LINE1 0001 001767 LL 0001 001764 LN 0001 001768 LI 0001 001416 MOLE
0001 000006 MOLES 0001 001772 N 0001 000007 NAME 0001 001754 NASH 0001 001753 NCOAL
0001 001747 MDUMMY 0001 001755 NFUEL 0001 001762 NI 0001 000017 NOF 0001 000020 NOMIT
0001 001756 NOXID 0001 000007 NP 0001 000011 NPT 0001 001745 NREAC 0001 000013 NS
0001 000010 NT 0001 003040 OFUEL 0001 001015 OMIT 0001 001751 OTEMP 0001 003242 OXID
0001 001365 PECVT 0001 000003 PER 0001 002727 PROX 0001 002002 PX 0001 000000 RDYES
0001 001632 RHOL 0001 001500 RTEMP 0001 004064 S 0001 001770 SINRT 0001 016460 SLN
0001 000004 SP 0001 015364 SUB 0001 001771 SUM 0001 001773 SUM1 0001 001775 SUM2
0001 002004 SUM3 0001 016514 TEMP 0001 000002 TP 0001 000002 WCR

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00101 1* SUBROUTINE COALCV(FIRST)
00101 2* USE MIPS INPUT ROUTINES TO READ COAL CONVERSION
00101 3* AND CREATE SIMULATED REACTANT CARDS
00103 4* COMMON /CFUEL/CF,HHVV,WCR,PER
00104 5* COMMON /SPECES/COEF(12,7,150),S(150),EM(150,13),ENLM(150),MO(150)
00104 6* X DELM(150),A(15,150),SUB(150,3),IUSE(150),TEMP(150,2),SLN(150)
00105 7* COMMON /IMDX/IDEBUG,CONVG,TP,HP,SP,ISV,MOLES,MP,NT,NPT,L,NS,
00105 8* X KMAT,IMAT,IQ1,NOF,NOMIT
00106 9* COMMON /CCC/GRAPH,JOUT,DEMAND
00107 10* INTEGER OMIT
00110 11* DIMENSION OMIT(3,50)
00111 12* EQUIVALENCE (OMIT(1,1),ENLM(1))
00112 13* LOGICAL FIRST,RDYES
00113 14* DIMENSION LINF(17)

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COALCV

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00214 71* 12 ICOAL(I,1)=ID(I) 000016
00215 72* FOR FIRST PASS DO NOT CHECK SAVED DATA 000016
00216 73* IF (NOT, FIRST) GO TO 10 000020
00220 74* IF (NOT, RDYES(LINE1,42)) GO TO 300 000022
00222 75* 10 CONTINUE 000030
00222 76* C READ IN PREVIOUS COAL DATA 000030
00223 77* REMIND IC 000030
00224 78* READ (IC) NDMY,CF,HVV,WCR,PER 000032
00233 79* READ (IC) CTMP,OTEMP 000043
00237 80* READ (IC) PROX,COAL,PER,IE,HM 000051
00246 81* READ (IC) NCOAL,NASH,MFUEL,NOXID 000071
00254 82* READ (IC) ICOMP(I,J),I=1,12,J=1,MCOAL, 000112
00254 83* X ((ACOMP(I,J),I=1,13),J=1,NASH), 000112
00254 84* X ((OFUEL(I,J),I=1,13),J=1,MFUEL), 000112
00254 85* X ((OXID(I,J),I=1,11),J=1,NOXID) 000112
00254 86* C DISPLAY PRESENT COAL DATA 000112
00312 87* IF (FIRST) GO TO 50 000150
00314 88* IF (NOT, RDYES(LINE1,42)) GO TO 300 000182
00316 89* 50 CONTINUE 000160
00317 90* CALL GOUTT(1 - VOLATILE (OPTIONAL) AND ASH AS LBS/100 LBS DRY COA 000160
00317 91* XL,56) 000160
00320 92* ENCODE (56,IOUT) PROX(1) 000163
00323 93* 56 FORMAT (6X,VOLATILE,F10.4) 000171
00324 94* CALL GOUTT(IOUT,24) 000171
00325 95* ENCODE (58,IOUT) PROX(3) 000175
00330 96* 58 FORMAT (6X,ASH,5X,F10.4) 000203
00331 97* CALL GOUTT(IOUT,24) 000203
00332 98* CALL GOUTT(1) 000207
00333 99* ENCODE (60,IOUT) CTMP 000213
00336 100* 60 FORMAT (1,2 - COAL TEMPERATURE IN DEG F,F10.2) 000221
00337 101* CALL GOUTT(IOUT,40) 000221
00340 102* CALL GOUTT(1) 000225
00341 103* CALL GOUTT(3 - DRY COAL COMPOSITION AS LBS/100 LBS DRY COAL,49) 000231
00342 104* DO 66 I=1,5 000240
00345 105* ENCODE (62,IOUT) ICOAL(I,1),COAL(I,2) 000246
00351 106* 62 FORMAT (5X,I4,5X,F10.4) 000246
00352 107* CALL GOUTT(IOUT,24) 000246
00353 108* 66 CONTINUE 000253
00355 109* CALL GOUTT(1) 000253
00356 110* CALL GOUTT(4 - OTHER COAL COMPONENTS AS LBS/100 LBS DRY COAL, STA 000257
00356 111* XTE AND COMPOSITION,73) 000257
00357 112* IF (INCOAL-EQ-0) GO TO 80 000263
00361 113* DO 72 I=1,NCOAL 000265
00364 114* ENCODE (70,IOUT) CCOMP(I,1),ICOMP(2,I), 000273
00364 115* X ((ICOMP(J*2+1,1),CCOMP(J*2+2,1),J=1,5) 000273
00375 116* 70 FORMAT (F10.4,10X,A4,512X,A2,2X,F8.4)) 000306
00376 117* CALL GOUTT(IOUT,94) 000306
00377 118* 72 CONTINUE 000316
00401 119* 80 CALL GOUTT(1) 000316
00402 120* CALL GOUTT(5 - ASH COMPOSITION AS LBS/100 LBS ASH AND COMPONENT, 000321
00402 121* X 53) 000321
00403 122* IF (NASH-EQ-0) GO TO 90 000327
00403 123* DO 88 I=1,NASH 000335
00410 124* ENCODE (84,IOUT) ACOMP(I,1), (IACOMP(J*2+1,1),J=1,5) 000335
00420 125* 88 FORMAT (F10.4,14X,5(2X,A2,2X,F8.4)) 000347
00421 126* CALL GOUTT(IOUT,94) 000347

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00422 127* 88 CONTINUE
00424 128* 90 CALL GOUT(' ',1)
00425 129* ENCODE (192,IOUT) PER
00430 130* 92 FORMAT (' A - FRACTION CARBON CONVERSION',F10.4)
00431 131* CALL GOUT(IOUT,41)
00432 132* CALL GOUT(' ',1)
00433 133* ENCODE (196,IOUT) MH(1E+1)
00436 134* 96 FORMAT (' 7 - HEATING VALUE OF COAL BTU/LB*,F13.3)
00439 135* CALL GOUT(IOUT,46)
00440 136* CALL GOUT(' ',1)
00441 137* CALL GOUT(' A - OTHER FUEL COMPONENTS AS LBS/LB COAL, TEMPERATURE
00441 138* XIN DEG F, STATE AND COMPOSITION',86)
00442 139* IF (NFUEL.EQ.0) GO TO 104
00444 140* DO 102 I=1,NFUEL
00447 141* ENCODE (100,IOUT) OFUEL(1,1),OFUEL(2,1),OFUEL(3,1),
00447 142* X (10,FUEL(J*2+1),OFUEL(J*2+3,1),J=1,5)
00461 143* 100 FORMAT (F10.4,F10.3,1X,A3,5(2X,A2,2X,F8.4))
00462 144* CALL GOUT(IOUT,94)
00463 145* 102 CONTINUE
00465 146* 104 CALL GOUT(' ',1)
00466 147* ENCODE (106,IOUT) OTEMP
00471 148* 106 FORMAT (' 9 - OXIDIZER TEMPERATURE IN DEG F.,F10.2)
00472 149* CALL GOUT(IOUT,44)
00473 150* CALL GOUT(' ',1)
00474 151* CALL GOUT(' 10 - OXIDIZER COMPONENTS AS LBS/100 LBS OXIDIZER AND C
00474 152* X COMPONENT',63)
00474 153* IF (NOXID.EQ.0) GO TO 112
00477 154* DO 110 I=1,NOXID
00502 155* ENCODE (108,IOUT) OXID(1,1),OXID(J*2,1),OXID(J*2+1,1),J=1,5)
00512 156* 108 FORMAT (F10.4,14X,5(2X,A2,2X,F8.4))
00513 157* CALL GOUT(IOUT,94)
00514 158* 110 CONTINUE
00516 159* 112 CALL GOUT(' ',1)
00517 160* CALL GOUT(' TYPE 1 OR 2 TO MODIFY OR REPLACE',33)
00520 161* CALL GOUT(' RETURN TO CONTINUE',23)
00521 162* IQPT=0
00522 163* 114 CONTINUE
00523 164* CALL PDAT(1,1,IOPT,5114)
00524 165* IF (IOPT.LT.0.OR.IOPT.GT.2) GO TO 114
00526 166* IF (IOPT.EQ.0) GO TO 680
00530 167* GO TO (120,300),IOPT
00530 168* C SELECT GROUPS TO BE CHANGED
00531 169* 120 CONTINUE
00532 170* DO 124 I=1,10
00535 171* 124 JOPT(I)=0
00537 172* CALL GOUT (' TYPE GROUP NUMBERS OF DATA TO BE CHANGED IN ASCENDING
00537 173* X ORDER, FOR EXAMPLE 1 3 7 9',83)
00540 174* 126 CONTINUE
00541 175* CALL PDAT(10,JOPT,5126)
00542 176* DO 130 I=10,1,-1
00545 177* JJ=JOPT(I)
00546 178* IF (JJ.EQ.0) GO TO 130
00550 179* JOPT(I)=0
00551 180* JOPT(JJ)=JJ
00552 181* 130 CONTINUE
00552 182* C ADD OR UPDATE COAL DATA

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00554 183* 300 CONTINUE
00555 184* CALL PAGIT
00556 185* IF (JOPT(1).EQ.0) GO TO 314
00557 186* READ IN PROXIMATE ANALYSIS DATA
00558 187* C
00559 188* 310 CALL GOUT(' TYPE (OPTIONAL) LBS VOLATILES/100 LBS DRY COAL',N7)
00560 189* CALL RDATAF(1,PROX(1),S101)
00561 190* IF (1,PROX(1),EQ.0) PROX(1)=0.
00562 191* 312 CALL GOUT(' TYPE LBS ASH/100 LBS DRY COAL',S0)
00563 192* CALL RDATAF(1,PROX(1),S12)
00564 193* PROX(2)=100.-PROX(1)-PROX(3)
00565 194* 314 IF (JOPT(2).EQ.0) GO TO 320
00566 195* READ IN COAL TEMPERATURE
00567 196* C
00568 197* 316 CALL GOUT(' TYPE COAL TEMPERATURE IN DEG F',S11)
00569 198* CALL RDATAF(1,CTEMP,S16)
00570 199* 320 IF (JOPT(3).EQ.0) GO TO 340
00571 200* READ IN REACTING COAL COMPOSITION
00572 201* C
00573 202* 322 CALL GOUT(' C',S2)
00574 203* CALL RDATAF(1,COAL(1,2),S322)
00575 204* 324 CALL GOUT(' H',S2)
00576 205* CALL RDATAF(1,COAL(2,2),S324)
00577 206* 326 CALL GOUT(' N',S2)
00578 207* CALL RDATAF(1,COAL(3,2),S326)
00579 208* 328 CALL GOUT(' O',S2)
00580 209* CALL RDATAF(1,COAL(4,2),S328)
00581 210* 330 CALL GOUT(' S',S2)
00582 211* CALL RDATAF(1,COAL(5,2),S330)
00583 212* 340 IF (JOPT(4).EQ.0) GO TO 350
00584 213* READ IN OTHER COAL COMPONENTS
00585 214* C
00586 215* CALL GOUT(' TYPE (OPTIONAL) OTHER COAL COMPONENTS',S38)
00587 216* CALL GOUT(' TYPE LBS/100 LBS DRY COAL, STATE AND COMPONENT',S50)
00588 217* CALL GOUT(' COAL TEMPERATURE IS ASSUMED',S28)
00589 218* NI=1
00590 219* 342 CALL GOUT(' EXAMPLE 0.13 IMG 2HCL 2.',S32)
00591 220* 343 DO 344 J=1,S
00592 221* ICOMP(J*2+1,NI)=2H
00593 222* 344 CCOMP(J*2+2,NI)=0.
00594 223* CCOMP(1,NI)=0.
00595 224* ICOMP(2,NI)=.
00596 225* 346 CALL RDATAF(12,CCOMP(1,NI),S342)
00597 226* IF (ICOMP(1,NI)) .348,
00598 227* IF (ICOMP(1,NI).EQ.0) GO TO 348
00599 228* NI=NI+1
00600 229* GO TO 343
00601 230* 348 NCOAL=NI-1
00602 231* 350 IF (JOPT(5).EQ.0) GO TO 380
00603 232* IF (JOPT.NE.1) GO TO 351
00604 233* ENCODE (2350,IOUT) JOPT(5)
00605 234* 2350 FORMAT (' GROUP NUMBER',I5)
00606 235* CALL GOUT(IOUT,18)
00607 236* 2352 IF (NASH.EQ.0) GO TO 2357
00608 237* DO 2356 I=1,NASH
00609 238* ENCODE (235N,IOUT) I,ACOMP(1,I),
00610 239* X IACOMP(J*2+1,I),IACOMP(J*2+1,I),J=1,5)
00611 240* 2354 FORMAT (14,F10.4,14X,5(2X,A2,2X,F8.4))
00612 241* CALL GOUT(IOUT,98)
00613 242* 238*
00614 243*
00615 244*
00616 245*
00617 246*
00618 247*
00619 248*
00620 249*
00621 250*
00622 251*
00623 252*
00624 253*
00625 254*
00626 255*
00627 256*
00628 257*
00629 258*
00630 259*
00631 260*
00632 261*
00633 262*
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00637 266*
00638 267*
00639 268*
00640 269*
00641 270*
00642 271*
00643 272*
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00656 285*
00657 286*
00658 287*
00659 288*
00660 289*
00661 290*
00662 291*
00663 292*
00664 293*
00665 294*
00666 295*
00667 296*
00668 297*
00669 298*
00670 299*

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00671 239* 2356 CONTINUE 001137
00673 240* 2357 CALL GOUTI* TYPE 1-ALTER, 2-DELETE, 3-ADD, RETURN TO CONTINUE*,50) 001137
00674 241* 2358 KOUT=0 001143
00675 242* 001143
00676 243* IF (KOUT.LT.0.OR.KOUT.GT.3) GO TO 2358 001150
00700 244* IF (KOUT.EQ.0) GO TO 2360 001165
00702 245* IF (KOUT.EQ.3) GO TO 2370 001167
00704 246* CALL GOUTI* TYPE LINE NUMBER*,17) 001172
00705 247* 2360 LN=0 001177
00706 248* CALL RDATAI(1,LN,2360) 001177
00707 249* IF (LN.LE.0.OR.LN.GT.NASH) GO TO 2360 001204
00711 250* IF (KOUT.EQ.1) GO TO 2366 001221
C 001221
00713 252* DELETE 001221
00714 253* L1=LN* 001224
00716 254* IF (LN.EQ.NASH) GO TO 2364 001227
00721 255* DO 2362 I=L1,NASH 001234
00724 256* DO 2362 J=1,11 001245
00725 257* ACOMP(J,I-1)=ACOMP(J,I) 001245
00730 258* 2362 CONTINUE 001250
00731 259* 2364 NASH=NASH-1 001250
00731 259* GO TO 2352 001252
00731 260* C 001254
00732 261* 2366 MI=LN 001254
00733 262* GO TO 2372 001255
C 001255
00733 263* ADD 001255
00734 264* 2370 NASH=NASH+1 001257
00735 265* NI=NASH 001261
00735 266* C 001261
00736 267* READ IN NEW DATA 001261
00737 268* 2372 CALL GOUTI* LBS/100 LBS DRY ASH AND COMPONENT*,34) 001263
00742 269* DO 2374 J=1,5 001266
00743 270* IACOMP(J*2,NI)=2H 001300
00745 271* ACOMP(J*2+1,NI)=0. 001301
00746 272* CALL RDATAF(1,ACOMP(1,NI),2372) 001303
00746 273* GO TO 2352 001313
C 001313
00747 274* CHECK FOR FES2 001315
00750 275* 2380 FES2=0. 001315
00753 276* DO 2386 I=1,NASH 001315
00756 277* DO 2384 J=1,5 001334
00760 278* IF (IACOMP(J*2,I)+NE-IASH(J*2-1,4)) GO TO 2386 001334
00762 279* IF (ACOMP(J*2+1,I)+NE-ASH(J*2,4)) GO TO 2386 001337
00764 280* 2384 CONTINUE 001346
FES2=ACOMP(1,I) 001346
GO TO 380 001350
00765 281* 2386 CONTINUE 001354
00766 282* GO TO 380 001354
00770 283* 351 CONTINUE 001356
C 001356
00771 284* READ IN ASH COMPONENTS 001356
00772 285* CALL GOUTI* TYPE LBS/100 LBS DRY ASH FOR COMPONENTS*,40) 001356
00773 286* CALL GOUTI* STATE ASSUMED SOLID, COAL TEMPERATURE ASSUMED*,47) 001361
00774 287* 352 CALL GOUTI* ST02*,5) 001366
00775 288* CALL RDATAF(1,ACOMP(1,1),3352) 001371
00776 289* 354 CALL GOUTI* FE203*,6) 001377
00777 290* CALL RDATAF(1,ACOMP(1,2),3354) 001402
00777 291* 356 CALL GOUTI* AL2O3*,6) 001410
00777 292* CALL RDATAF(1,ACOMP(1,3),3356) 001417
00777 293* 358 CALL GOUTI* FES2*,5) 001421
00777 294* 001421

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01001 295* CALL RDATAF(1,ACOMP(1,4),5358) 001424
01002 296* FES2=ACOMP(1,4) 00143
01005 297* IF (IACOMP(1,4).EQ.* ) FES2=0. 001433
01007 298* J=0 001437
01007 299* REMOVE ANY ZERO COMPONENTS 001437
01010 300* DO 364 I=1,N 001444
01013 301* IF (IACOMP(1,I)) 364. 001450
01016 302* IF (IACOMP(1,I).EQ.* ) GO TO 364 001452
01020 303* J=J+1 001455
01021 304* ACOMP(1,J)=ACOMP(1,I) 001461
01022 305* IF (I.NE.J) ACOMP(1,I)=0. 001462
01024 306* DO 362 LL=1,10 001466
01027 307* 362 ACOMP(LL+1,J)=ASHILL(I) 001477
01031 308* 364 CONTINUE 001504
01033 309* NI=J+1 001504
01033 310* C ADD OTHER ASH COMPONENTS 001504
01034 311* CALL GOUT(' CONTINUE WITH ASH COMPONENTS',29) 001507
01035 312* CALL GOUT(' LBS/100 LBS DRY ASH AND COMPONENTS',34) 001513
01036 313* 366 CALL GOUT(' EXAMPLE 0.25 ZHTI 1. 1MO 2. 38) 001520
01037 314* 367 DO 368 J=1,5 001524
01042 315* IACOMP(J+2,NI)=2H 001535
01043 316* 368 ACOMP(J+2+1,NI)=0. 001536
01045 317* 370 CALL RDATAF(11,ACOMP(1,NI),5366) 001540
01046 318* IF (IACOMP(1,NI)) 372, 001550
01051 319* IF (IACOMP(1,NI).EQ.* ) GO TO 372 001552
01053 320* NI=NI+1 001555
01054 321* GO TO 367 001560
01055 322* 372 NASH=NI-1 001562
01056 323* 380 IF (JOPT(4).EQ.0) GO TO 390 001565
01056 324* C READ COAL CONVERSION FRACTION 001567
01060 325* 382 CALL GOUT(' TYPE CARBON CONVERSION FRACTION, FOR EXAMPLE, 0.89', 001572
01061 326* X 51) 001572
01061 327* CALL RDATAF(1,PER,5382) 001572
01061 328* C COMPUTE VALUES FOR HHV BY DIFFERENT FORMULAS 001572
01062 329* 390 CONTINUE 001572
01063 330* HH(2)=145.44*COAL(1,2)+620.28*(COAL(2,2)-0.125*COAL(4,2)) 001600
01063 331* X +0.50*COAL(5,2) 001600
01064 332* HH(3)=146.0*COAL(1,2)+620.0*(COAL(2,2)-0.125*COAL(4,2)) 001614
01064 333* X +0.50*COAL(5,2) 001614
01065 334* HH(4)=144.9*COAL(1,2)+610.0*(COAL(2,2)-0.125*COAL(4,2)) 001623
01065 335* X +55.50*COAL(5,2) 001623
01066 336* HH(5)=1654.3*COAL(2,2)/(100.-PROX(3))+424.62)* 001634
01066 337* X (COAL(1,2)/3.+COAL(2,2)-0.125*COAL(4,2)-COAL(5,2)) 001634
01067 338* HH(6)=146.58*COAL(1,2)+568.78*COAL(2,2)+29.4*COAL(5,2) 001653
01067 339* X -6.58*PROX(3)-51.53*(COAL(3,2)+COAL(4,2)) 001653
01070 340* HH(7)=AMAX1(HH(2),HH(3),HH(4),HH(5),HH(6)) 001673
01071 341* HH(8)=AMIN1(HH(2),HH(3),HH(4),HH(5),HH(6)) 001715
01072 342* DO 392 I=2,8 001743
01075 343* ENCODE (394,HH(I*5-1)) HH(I) 001743
01100 344* 392 CONTINUE 001753
01102 345* 394 FORMAT (F12.3) 001753
01103 346* IF (JOPT(7).EQ.0) GO TO 420 001753
01105 347* CALL GOUT(' HHV CALCULATION',16) 001755
01106 348* DO 398 I=1,8 001764
01111 349* CALL GOUT(HH(I*5-4),30) 001764
01112 350* 398 CONTINUE 001773

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01114 351* 400 CALL RDATA1(1,IE,5400) 001773
01115 352* IF (IE.LT.D-OR.IE-51.8) GO TO 400 001777
01117 353* IF (IE.GT.D) GO TO 420 002014
01121 354* 402 CALL GOUT1* ENTER HHV AS BTU/LB COAL*, 25) 002020
01122 355* CALL RDATA1(1,HH(1),5402) 002023
01123 356* HHV=HH(IE+1) 002031
01124 357* IF (JOPT(8),EQ,0) GO TO 440 002033
01126 358* IF (IOPT,NE,1) GO TO 421 002035
01130 359* ENCODE (2350,IOUT), JOPT(8) 002040
01133 360* CALL GOUT(IOUT,18) 002046
01134 361* 2420 IF (MFUEL=EQ,0) GO TO 2427 002053
01136 362* DO 2426 I=1,NFUEL 002054
01141 363* ENCODE (244,4,IOUT) 1,OFUEL(1,1),OFUEL(2,1),OFUEL(3,1), 002063
01141 364* X 1,OFUEL(J*2+2,1),OFUEL(J*2+3,1),J=1,5 002063
01154 365* 2424 FORMAT (14,F10.4,F10.3,1X,A3,5(2X,A2,2X,F8.4)) 002101
01155 366* CALL GOUT(IOUT,98) 002101
01156 367* 2426 CONTINUE 002112
01160 368* 2427 CALL GOUT1* TYPE 1-ALIER, 2-DELETE, 3-ADD, RETURN TO CONTINUE*,50) 002112
01161 369* 2422 KOUT=0 002116
01162 370* CALL RDATA1(1,KOUT,52422) 002116
01163 371* IF (KOUT.LT.D-OR.KOUT-61.3) GO TO 2422 002123
01165 372* IF (KOUT=EQ,0) GO TO 430 002140
01167 373* IF (KOUT=EQ,3) GO TO 2434 002142
01171 374* CALL GOUT1* TYPE LINE NUMBER*,17) 002145
01172 375* 2428 LN=0 002152
01173 376* CALL RDATA1(1,LN,52428) 002152
01174 377* IF (LN.LT.D-OR.LN-61.NFUEL) GO TO 2428 002157
01176 378* IF (KOUT=EQ,1) GO TO 2432 002174
01176 379* C DELETE 002174
01200 380* LI=LN+1 002177
01201 381* IF (LN=EQ,NFUEL) GO TO 2431 002202
01203 382* DO 2430 I=1,NFUEL 002205
01206 383* DO 2430 J=1,13 002213
01211 384* OFUEL(J,I-1)=OFUEL(J,I) 002213
01212 385* 2430 CONTINUE 002216
01215 386* 2431 NFUEL=NFUEL-1 002216
01216 387* GO TO 2420 002220
01216 388* C ALTER 002220
01217 389* 2432 NI=LN 002222
01220 390* GO TO 2436 002223
01220 391* C ADD 002223
01221 392* 2434 NFUEL=NFUEL+1 002225
01222 393* NI=NFUEL 002227
01222 394* C READ IN NEW DATA 002227
01223 395* 2436 CALL GOUT1* TYPE LBS/LB COAL, TEMPERATURE (DEG F) AND STATE AND CO 002231
01223 396* XMPONENT*,63) 002231
01224 397* DO 2438 I=1,5 002234
01227 398* 1,OFUEL(J*2+2,NI)=2H 002246
01230 399* 2438 OFUEL(J*2+3,NI)=0. 002247
01232 400* OFUEL(1,NI)=0. 002251
01233 401* OFUEL(2,NI)=0. 002253
01234 402* 1,OFUEL(3,NI)= 002254
01235 403* CALL RDATA1(13,OFUEL(1,NI),52436) 002256
01236 404* GO TO 2420 002265
01237 405* 421 CONTINUE 002267
01237 406* C READ IN OTHER FUEL COMPONENTS 002267

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002261 CALL GOUT(' TYPE OTHER FUEL COMPONENTS',27)
002272 CALL GOUT(' TYPE LBS/LB COAL, TEMPERATURE (DEG F) AND STATE AND CO
002273 COMPONENT',63)
002276 NI=1
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01360 46.0 SUM1=0.
01361 46.0 DO 486 I=1,5
01362 46.0 ANUMIN,I)=ANUMIN,I)/PMOL(I)
01363 46.0 SUM1=SUM1+ANUMIN,I)
01364 46.0 DO 486 I=1,5
01365 46.0 ANUMIN,I)=ANUMIN,I)/SUM1*100.
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01473 519* 508 CONTINUE
01475 520* 520 NREAC=NREAC+N*UAL
01476 521* C CREATE CARDS FOR ASH COMPONENTS
01477 522* N=NREAC
01478 523* SUM2=0
01479 524* IF (1.5H*EQ.0) GO TO 548
01500 525* ASHF=CF*PROX(1)/100
01501 526* DO 522 I=1,NASH
01502 527* SUM2=SUM2+ACOMP(1,I)
01503 528* DO 528 I=1,NASH
01504 529* DO 526 J=1,5
01505 530* NAMEIN(I,J)=IACOMP(J*2,I)
01506 531* 526 / UM(N+1,J)=ACOMP(J*2,I)
01507 532* PC*WT(N+1)=IACOMP(1,I)*ASHF)/SUM2
01508 533* MOLE(N+1)=1H
01509 534* FAZ(N+1)=1H5
01510 535* ENTH(N+1)=0
01511 536* NAMEIN(I,6)=2400
01512 537* ANUM(N+1,6)=0
01513 538* RTEMP(N+1)=(CTEMP-32.)/1.8+273.15
01514 539* FOX(N+1)=1HF
01515 540* DENSIN(I)=0
01516 541* 528 CONTINUE
01517 542* 540 NREAC=NREAC+NASH
01518 543* C COMPUTE ENTHALPY FOR COAL
01519 544* FES2=FES2+ASHF/(SUM2*CF)
01520 545* HHV=((HHVV-14485.7*51NRT/100.)/1.8)*(100./SUM1)+(100./SUM1)*100.
01521 546* FES2C=(100./1.8+119.85)*(100./SUM1)+(100./SUM1)*FES2
01522 547* HF1=-ANUM(NS,1)*94051.8-0.5*ANUM(NS,2)*68317.4
01523 548* X -ANUM(NS,5)*70960.-FES2C*197650.
01524 549* PX=100.*PROX(1)/(PROX(1)+PROX(2))
01525 550* HF2=(1.75*(CTEMP-77)+.0029*PX*(CTEMP-77))*
01526 551* X 0.00025*(CTEMP-60)*2-0.07225*(100./SUM1)+(100./SUM1)*1.8
01527 552* ENTH(NS)=HHV*HF1+HF2
01528 553* C CREATE CARDS FOR OTHER FUEL COMPONENTS
01529 554* N=NREAC
01530 555* IF (NFUEL.EQ.0) GO TO 560
01531 556* DO 548 I=1,NFUEL
01532 557* DO 546 J=1,5
01533 558* NAME(N+1,J)=IOFUEL(J*2+2,I)
01534 559* ANUM(N+1,J)=OFUEL(J*2+3,I)
01535 560* PECUT(N+1)=OFUEL(1,I)*CF
01536 561* MOLE(N+1)=1H
01537 562* IFAZ(N+1)=IOFUEL(3,I)
01538 563* ENTH(N+1)=0
01539 564* NAME(N+1,6)=2400
01540 565* ANUM(N+1,6)=0
01541 566* RTEMP(N+1)=(OFUEL(2,I)-32.)/1.8+273.15
01542 567* FOX(N+1)=1HF
01543 568* DENSIN(I)=0
01544 569* 548 CONTINUE
01545 570* C LOOK UP CARBON
01546 571* DO 552 I=1,NFUEL
01547 572* DO 550 J=1,5
01548 573* IF (NAMEIN(I,J).NE.ICC(J)) GO TO 552
01549 574* IF (ANUM(N+1,J)-CC(J)) 552,552

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01606 575* 550 CONTINUE
01610 576* GO TO 55*
01611 577* 552 CONTINUE
01613 578* GO TO 560
01613 579* C CREATE INERT CARBON CARD FOR RECYCLE CARBON
01614 580* 55* DO 55* J=1,6
01617 581* NAME(N,NFUEL,I,J)=NAME(N,I,J)
01620 582* ANUM(N,NFUEL,I,J)=ANUM(N,I,J)
01622 583* NAME(N,NFUEL,I,J)=,IC
01623 584* PECWT(N,NFUEL,I,J)=,PER*PECWT(N,I)
01624 585* PECWT(N,I)=PER*PECWT(N,I)
01625 586* MOLE(N,NFUEL,I,J)=MOLE(N,I)
01626 587* FAZ(N,NFUEL,I,J)=FAZ(N,I)
01627 588* ENTH(N,NFUEL,I,J)=ENTH(N,I)
01630 589* RTEMP(N,NFUEL,I,J)=RTEMP(N,I)
01631 590* FOX(N,NFUEL,I,J)=FOX(N,I)
01632 591* DENS(N,NFUEL,I,J)=DENS(N,I)
01633 592* NREAC=NREAC,I
01634 593* 560 NREAC=NREAC,NFUEL
01634 594* C CREATE CARDS FOR OXIDIZER COMPONENTS
01635 595* N=NREAC
01636 596* IF (NOXID.EQ.0) GO TO 590
01640 597* SUM3=0.
01641 598* DO 572 I=1,NOXID
01644 599* 572 SUM3=SUM3+OXID(I,I)
01646 600* DO 576 I=1,NOXID
01651 601* DO 576 J=1,5
01654 602* NAME(N,I,J)=NOXID(J*2,I)
01655 603* ANUM(N,I,J)=OXID(J*2+1,I)
01657 604* PECWT(N,I)=OXID(I,I)/SUM3
01660 605* MOLE(N,I)=1H
01661 606* FAZ(N,I)=1H6
01662 607* ENTH(N,I)=0.
01663 608* NAME(N,I,6)=2H00
01664 609* ANUM(N,I,6)=0.
01666 610* RTEMP(N,I)=(OTEMP-32.)/1.8+273.15
01666 611* FOX(N,I)=1H0
01667 612* DENS(N,I)=0.
01670 613* 578 CONTINUE
01672 614* 590 NREAC=NREAC+NOXID
01673 615* C SAVE COAL DATA
01673 616* COAL(1,2)=COAL(1,2)/PER
01674 617* REMIND IC
01675 618* WRITE (IC) NREAC,CF,HHV,WCP,PER
01676 619* WRITE (IC) CTEMP,OTEMP
01677 620* WRITE (IC) PROX,COAL,PER,IE,HH
01678 621* WRITE (IC) NCOAL,NASH,NFUEL,NOXID
01679 622* WRITE (IC) (ICOMP(I,J),I=1,12),J=1,NCOAL,
01680 623* X (ICOMP(I,J),I=1,11),J=1,NASH,
01681 624* X (IOFUEL(I,J),I=1,13),J=1,NFUEL,
01682 625* X (IOXID(I,J),I=1,11),J=1,NOXID
01683 626* C WRITE OUT REACTANT FILE
01684 627* WRITE (IC) NREAC,CF
01685 628* DO 610 I=1, NREAC
01686 629* WRITE (IC) (NAME(I,J),ANUM(I,J),J=1,5),PECWT(I),MOLE(I),
01687 630* X ENTH(I),NAME(I,6),ANUM(I,6),FAZ(I),RTEMP(I),FOX(I),DENS(I)

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02012	631*	610	CONTINUE	003646
02014	632*	END	FILE IC	003646
02015	633*	680	CONTINUE	003652
02016	634*		RETURN	003652
02017	635*		END	003712

END OF COMPILATION: NO DIAGNOSTICS.

AMDG,P CPHS

FOR.S CPHS,CPHS
HSA E3 -10/15/80-13:06:13 (11.)

SUBROUTINE CPHS ENTRY POINT 000567

STORAGE USED: CODE(1) 000603; DATA(0) 000160; BLANK COMMON(2) 000000

COMMON BLOCKS:

0003 SPECES 017106
0004 MISC 001701
0005 INDX 000041
0006 LOWTH 001201
0007 CCC 000003

EXTERNAL REFERENCES (BLOCK, NAME)

0010 NWDS
0011 NI028
0012 ALOG
0013 NI015
0014 MERR38

STORAGE ASSIGNMENT (BLOCK, TYPE, RELATIVE LOCATION, NAME)

0001	000031	10L	0001	000207	1716	0001	000217	1745	0001	000093	20L	0001	000351	2216
0001	000062	254G	0001	000065	30L	0001	000067	31L	0001	00157	32L	0000	000041	333F
0001	000164	40L	0001	000176	60L	0001	000230	70L	0001	000233	80L	0001	000412	87L
0000	000060	88F	0001	000472	89L	0001	000531	90L	0000	000103	904F	0003	011052	A
0004	000640	AM	0004	000705	AM1	0004	001135	ANUM	0004	000004	ATOM	0004	000514	B0
0004	000545	BOP	0005	000036	CALCH	0005	000000	COEF	0005	000001	CONVG	0006	R 000361	CPL
0004	000706	CPR1	0004	R 000634	CPSUM	0000	R 000040	CPUSEO	0000	R 000035	CPX	0000	R 000007	CPXX
0004	000654	DATA	0003	010624	DELM	0007	000002	DEMAND	0004	001560	DEMS	0003	R 004312	EN
0003	010150	ENLN	0004	001700	ENLSAV	0004	000000	ENN	0004	001676	ENNL	0004	001677	ENSAVE
0004	001414	ENTH	0004	000636	EGRAT	0004	001445	FAZ	0004	001527	FOX	0007	000000	GRAPH
0006	R 000551	HL	0005	000003	HP	0004	000642	HPP	0004	000637	HSUBO	0000	P 000034	HX
0000	R 000013	HXX	0003	R 010376	HO	0000	I 000037	I	0005	000030	IC	0005	000000	IDEBUG
0000	I 000001	IER	0000	I 000023	IEXTND	0006	I 001131	ILSP	0005	000015	IMAT	0000	I 000002	IMSG
0005	000132	INJPS	0005	000023	IONS	0005	000021	IP	0005	000037	IOSAVE	0005	000016	IOI
0005	000003	ISV	0003	000034	IT	0003	I 016266	IUSE	0000	I 000026	IX	0005	I 000031	J
0005	000026	JLIQ	0007	I 000001	JOUT	0005	000025	J50L	0000	I 000024	K	0000	I 000025	KK
0005	000014	KMAT	0000	I 000027	KX	0004	000463	LLMT	0005	000040	LSAVE	0000	I 000036	M
0005	000006	MOLES	0004	000707	NAME	0005	000024	NC	0005	000022	NEWR	0005	000035	NFZ
0005	000012	NLM	0006	I 000000	NLTSP	0005	000017	NOF	0005	000020	NOMIT	0005	000007	NP
0005	I 000011	NPT	0005	000027	NREAC	0005	I 000013	NS	0000	I 000000	NSPPI	0005	000010	NT
0000	I 000030	NTUP	0004	000635	OF	0004	001644	OYF	0004	001363	PECWT	0004	000633	PP
0004	000644	PH	0004	001611	RHOP	0004	001612	RMW	0004	001476	RTEMP	0003	R 004064	S
0005	000033	SHOCK	0006	R 000741	SL	0003	016660	SLN	0005	000004	SP	0003	I 015364	SUB
0006	I 000001	SU3LT	0004	000001	SUMN	0000	R 000033	SX	0000	R 000017	SXX	0004	000003	SO
0003	016514	TEMP	0004	000632	THIGH	0006	R 000171	TL	0004	R 001643	TLN	0000	R 000032	TLS
0004	R 000640	TLOW	0004	000627	TM	0004	R 000631	TMID	0005	000002	TP	0004	R 000002	TT
0000	R 000031	TTS	0000	R 000003	TXA	0004	000646	VMIN	0005	000032	VOL	0004	000650	VPLS

000* 000652 WP

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00101 1* SUBROUTINE CPHS
00101 2* C
00101 3* C
00101 4* C
00101 5* C
00101 6* C
00101 7* C
00101 8* C
00101 9* C
00101 10* C
00101 11* C
00101 12* C
00101 13* C
00101 14* C
00101 15* C
00101 16* C
00101 17* C
00101 18* C
00101 19* C
00101 20* C
00101 21* C
00101 22* C
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00101 33* C
00101 34* C
00101 35* C
00101 36* C
00101 37* C
00101 38* C
00101 39* C
00101 40* C
00101 41* C
00101 42* C
00101 43* C
00101 44* C
00101 45* C
00101 46* C
00101 47* C
00101 48* C
00101 49* C
00101 50* C
00101 51* C

SUBROUTINE CPHS
CALCULATES THERMODYNAMIC PROPERTIES FOR INDIVIDUAL SPECIES

COMMON /SPECES/ COEF(2,7,150),S(150),EM(150,13),ENL(150),H(150)
1,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2),SLN(150)
INCLUDE SPECPX
COMMON /MISC/ ENN,SUMN,TT,SO,ATOM(3,101),LLMT(25),BO(25),
BO(25,2),TM,TLOW,TMID,TWIGH,PP,CPSUM,OF,EQRAT,
HSURD,AM(2),HPP(2),RH(2),VMIN(2),VPLS(2),WP(2),
DATA(25),AMI,CPRI,NAME(25,6),ANUM(25,6),PECWT(25),
ENTH(25),FAZ(25),RTEMP(25),FOX(25),DEMS(25),RHOP,
RMW(25),TLN,OXE(26),ENL+ENG+V+E+ENLSAV
COMMON /INDX/ IDEBUG,CONVG,TP,MP,SP,ISV,MOLFS,MP,NT,NPT,NLM,MS,
KMAT,IMAT,IO,MOF,NOMIT,IP,NEUR,IONS,NC,JSOL,LTQ,
NREAC,IC,J,VOL,SHOCK,IT,NFZ,CALCH,IOSAVE,LSAVE
COMMON /LWTH/ NLISP,SUBLT(40,3),TL(40,3),CPL(40,3),HL(40,3),
SL(40,3),ILSP(40)

COMMON /CCC/ GRAPH,JOUT,DEMAND
DATA IER/O',IMSG/-1/
DIMENSION TXX(4),CPXX(4),HXX(4),SXX(4)
INTEGER SUB,SUBLT

TEXTND = 0
IF(TT,LT,TLOW) TEXTND = 1
IF(EXTND.NE.O) IMSG = IMSG + 1
IF(IMG.NE.O) GO TO 10
IF(EXTND.NE.O) WRITE(JOUT,3333) TT
3333 FORMAT (//25X,8BLOW TEMPERATURE THERMO EXTENSION IN CPHS AT TT =,
1 F12.6,15H DEGREES KELVIN//)
10 K = 1
IF(TT,LE,TMID) K=2
KK=0
CPSUM=0
20 IF(COEF(K,1,J).NE.O) GO TO 30
IF(IUSE(J).LT.O) GO TO 40
KK=K
K=1
IF(KK.EQ.1) K=2
30 IF(EXTND.NE.O) GO TO 60
31 S(J) = ((COEF(K,5,J)/4.O)*TT + COEF(K,9,J)/3.O)*TT + COEF(K,3,J)
1/2.O)*TT + COEF(K,2,J)*TT + COEF(K,1,J)*TLN + COEF(K,7,J)
H(J) = ((COEF(K,5,J)/5.O)*TT + COEF(K,4,J)/4.O)*TT + COEF(K,3,J)/3.O)*TT
1+COEF(K,2,J)/2.O)*TT + COEF(K,1,J)*COEF(K,6,J)/TT
CPSUM=CPSUM+((COEF(K,5,J)*TT+COEF(K,4,J)*TT+COEF(K,3,J)*TT+COEF(K,2,J)*TT+COEF(K,1,J)*TLN+COEF(K,7,J))
IF(K,2,J))*TT+COEF(K,1,J))*ENH(J,NPT)
32 IF(KK.EQ.O) GO TO 40
KK=K
KK=0
40
41
42
43
44
45
46
47
48
49
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CPHS      DATE 101580
00162      52*      40 IF (J .EQ. NS) RETURN
00164      53*      J=J+1
00165      54*      GO TO 20
00166      55*      60 IF (NLTSP .EQ. 0) GO TO 31
00167      56*      DO 70 I=1,NLTSP
00170      57*      DO 65 KX=1,3
00171      58*      65 IF (SUB(J,KX) .NE. SUB(TIX,KX)) GO TO 70
00172      59*      GO TO 80
00173      60*      70 CONTINUE
00174      61*      GO TO 3
00175      62*      60 NTUP = 1LSP(IX)
00176      63*      IF (TIL-IL(IX,1)) GO TO 90
00177      64*      TTS = TT
00178      65*      TLN= TLN
00179      66*      TT = TLOW
00180      67*      TLN= ALOGITTI
00181      68*      KX = 2
00182      69*      SX = IL(COEF(KX,5,J)/4.)*TT+COEF(KX,4,J)/3.)*IL(COEF(KX,3,J)/2.)*
00183      70*      1.)*TT+COEF(KX,2,J))*TT+COEF(KX,1,J))*TLN+COEF(KX,7,J)
00184      71*      HX = IL(COEF(KX,5,J)/5.)*TT+COEF(KX,4,J)/4.)*TT+COEF(KX,3,J)/3.)*
00185      72*      1.)*TT+COEF(KX,2,J)/2.)*TT+COEF(KX,1,J))*COEF(KX,6,J)/TT
00186      73*      CPX= IL(COEF(KX,5,J))*TT+COEF(KX,4,J))*TT+COEF(KX,3,J))*TT
00187      74*      1.)*COEF(KX,2,J))*TT+COEF(KX,1,J)
00188      75*      DO 86 KX=1,NTUP
00189      76*      TTX(KX) = TL(IX,KX)
00190      77*      CPX(KX) = CPL(IX,KX)
00191      78*      HXX(KX) = HL(IX,KX)
00192      79*      86 SXX(KX) = SL(IX,KX)
00193      80*      TTX(NTUP+1) = TT
00194      81*      CPX(NTUP+1) = CPX
00195      82*      HXX(NTUP+1) = HX
00196      83*      SXX(NTUP+1) = SX
00197      84*      TT = TTS
00198      85*      TLN = TLN
00199      86*      M = 1
00200      87*      I = 1
00201      88*      IF (TT .LT. TTX(M)) I = -1
00202      89*      87 IF (TT .GE. TTX(M) .AND. TT .LE. TTX(M+1)) GO TO 89
00203      90*      M = M + 1
00204      91*      IF (M .LT. NTUP + 1 .AND. M .GT. 0) GO TO 87
00205      92*      WRITE (JOUT,88) TT,M,NTUP,(I,TTX(I), I=1,4)
00206      93*      FORMAT (//50X,29#CPHS= VARIABLE OUTSIDE TABLE//45X,4HTT =,1PE15.8
00207      94*      1,5H M =,12,8H NTUP =,12//50X,4HTTX(,11,3H) =,E15.8)
00208      95*      GO TO 31
00209      96*      89 SJU = SXX(M) + (SXX(M+1)-SXX(M))*((TT-TTX(M))/(TTX(M+1)-TTX(M))
00210      97*      HOUJ = HXX(M) + (HXX(M+1)-HXX(M))*((TT-TTX(M))/(TTX(M+1)-TTX(M))
00211      98*      CPUSD = CPX(M) + (CPX(M+1)-CPX(M))*((TT-TTX(M))/(TTX(M+1)-TTX(M))
00212      99*      CPSUM = CPSUM + CPUSD * EN(J,MPT)
00213      100*      GO TO 32
00214      101*      90 IF (IER .LT. 1) WRITE (JOUT,904) TT
00215      102*      904 FORMAT (//25X,60#ERROR DURING LOW TEMPERATURE THERMO EVALUATION IN
00216      103*      1 CPHS, TT =,F12.6,15H DEGREES CELVIN//)
00217      104*      IER = 1
00218      105*      GO TO 31
00219      106*      END
000164      CPHS 460
000171      CPHS 470
000174      CPHS 470
000176      CPHS 500
000177      CPHS 500
000217      CPHS 540
000226      CPHS 550
000231      CPHS 560
000231      CPHS 560
000233      CPHS 590
000238      CPHS 600
000241      CPHS 610
000243      CPHS 620
000245      CPHS 630
000247      CPHS 640
000253      CPHS 650
000255      CPHS 660
000255      CPHS 670
000301      CPHS 680
000301      CPHS 690
000325      CPHS 700
000325      CPHS 700
000351      CPHS 770
000351      CPHS 780
000352      CPHS 790
000354      CPHS 800
000356      CPHS 820
000361      CPHS 830
000363      CPHS 830
000365      CPHS 830
000367      CPHS 830
000371      CPHS 830
000373      CPHS 830
000375      CPHS 830
000377      CPHS 830
000400      CPHS 940
000412      CPHS 950
000430      CPHS 950
000433      CPHS 950
000450      CPHS 950
000470      CPHS 950
000470      CPHS 950
000472      CPHS 950
000472      CPHS 950
000506      CPHS 950
000514      CPHS 950
000522      CPHS 950
000527      CPHS 950
000531      CPHS 950
000542      CPHS 950
000542      CPHS 950
000542      CPHS 950
000544      CPHS 950
000602      CPHS 950

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CPHS

END OF COMPILATION: NO DIAGNOSTICS.

HDG,P DETON

DATE 101500

PAGE

ORIGINAL PAGE IS
OF POOR QUALITY

DETOM

2 FOR S DE ON DETOM
HSA C3 -10/15/80-13:06:18 (12.)

SUBROUTINE DETOM ENTRY POINT 001331

STORAGE USED: CODE(1) 001347; DATA(0) 000201; BLANK COMMON(2) 000000

COMMON BLOCKS:

0003 COMSIS 000006
0004 HOLCON 000010
0005 POINTS 000335
0006 MISC 001701
0007 INDX 000041
0010 PERF 000166
0011 OUP1 000073
0012 CCC 000003

EXTERNAL REFERENCES (BLOCK, NAME)

0013 NEWOF
0014 HCALC
0015 OUT1
0016 EQLBRM
0017 OUT2
0020 OUT3
0021 SAVE
0022 NWDUS
0023 NI025
0024 XPRR
0025 EXP
0026 SORT
0027 NI015
0030 NI035
0031 NERP35

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STORAGE ASSIGNMENT (BLOCK, TYPE, RELATIVE LOCATION, NAME)

0001	001305	1000L	0000	000035	11F	0001	000005	1306	0001	000040	146G	0001	000566	150L
0001	000053	154G	0000	000044	190F	0000	000053	203F	0001	000255	205L	0001	000176	214G
0000	000055	30F	0001	000651	341G	0001	000672	352G	0001	000711	362G	0001	000717	367G
0001	000563	40L	0001	000750	401G	0001	000767	411G	0001	001004	422G	0001	001024	433G
0001	001055	451G	0000	000114	46F	0001	001100	464G	0001	001115	475G	0000	000102	5F
0001	001123	502G	0001	001142	514G	0001	001157	525G	0001	001176	535G	0001	001216	546G
0000	000120	54F	0000	000123	68F	0001	000016	7L	0001	000615	860L	0000	000130	868F
0001	001251	870L	0001	001270	902L	0000	000032	ALAM	0000	000017	ALFA	0006	000640	AM
0006	000705	AM1	0006	001135	ANUM	0010	000133	APP	0003	000000	ATMN	0006	000004	AYOM
0000	000022	A11	0000	000023	A2	0000	000024	A21	0000	000025	A22	0006	000514	BO
0006	000545	80P	0000	000026	B1	0000	000027	B2	0007	000036	CALCH	0007	000001	CONVG
0006	000654	CP	0005	000032	CPR	0006	000706	CPR1	0006	000634	CPSUM	0012	000002	DEMAND
0006	001560	OENS	0005	000044	OLVPT	0005	000047	DLVTP	0004	000000	END	0006	001700	ENLSAV
0006	000000	ENN	0006	001676	ENNL	0006	001677	ENSAVE	0006	001414	ENTH	0010	000165	EOL

DETON

DATE 101580

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00111 24*      3      TWO*ZFROF      /OUPY/      000000
00111 25*      C      COMMON /CCC/ GRAPH,JOUT,DEMAND      000000
00112 26*      C      LOGICAL EQL,MP,TP      000000
00113 27*      DATA FG,SGHGA,MM1,FM,MM,MM,M1,FP1,6HP1,ATM,FP,6HP,P1, /      000000
00114 28*      1 FRA/6HP/0/RH,FRB,6HO1 /,FTT/6HT/TT /,FUD/6HDET VE/      000000
00114 30*      C      XX(A,X,B,Y,C,D) = (A*X-B*Y)/(A+C-R*D)      000000
00125 32*      C      IOF = 0      000000
00126 33*      DQ 4 11 = 1,AREAC      000000
00127 35*      4 NAME(11,6)=1ZERO      000005
00132 36*      TT = 0.      000007
00134 37*      IF (TT) .LE. 0.0) T(1) = RTMP(1)      000010
00135 38*      7 IOF = IOF+1      000016
00137 39*      OF = OF*(IOF)      000021
00140 40*      CALL MEMOF      000023
00141 41*      WRITE(JOUT,11)      000025
00142 42*      11 FORMAT(3H,DETONATION VELOCITY CALCULATIONS)      000032
00144 43*      DO 902 IF = 1,NT      000032
00145 44*      TT = T(1)      000040
00150 45*      CALL HCALL      000042
00151 46*      CALL OUT1      000044
00152 47*      DO 902 IF=1,MP      000046
00153 48*      H1(NPT) = RBAR*HSUBO      000055
00156 49*      TUB(NPT) = T(1)      000061
00157 50*      PUB(NPT) = P(1)      000063
00160 51*      CP(NPT) = RBAR*CPRI      000065
00161 52*      ITR = 0      000070
00162 53*      TT = 3500.      000071
00163 54*      PP = 15.      000073
00164 55*      PP = PP*(1)      000075
00165 56*      HSUBO = H1(NPT)/RBAR * 0.750*(1+PP/AM1      000077
00166 57*      IP = .FALSE.      000105
00167 58*      HPE = .TRUE.      000106
00170 59*      CALL EGLBHM      000110
00171 60*      HSUBO = H1(NPT)/RBAR      000117
00172 61*      HPE = .FALSE.      000122
00173 62*      IF (TT .LE. 0.0) GO TO 902      000123
00174 63*      GAM = GAMMA(NPT)      000126
00176 64*      TTI = TT/T(1)      000131
00177 65*      IIE = 0      000132
00200 66*      TEM=11-.75*PP1/(CPR(NPT)*AM1)      000143
00201 67*      WRITE(JOUT,190)TT      000150
00205 68*      190 FORMAT(8H,EST.=,F8.2/11X,4HP/P1,17Y,4HT/TT)      000160
00206 70*      WRITE(JOUT,203) 11,PP1,TT1      000160
00213 71*      DO 202 II = 1,3      000176
00216 72*      ALFA = MM(NPT)/AM1/TT1      000176
00217 73*      PP1 = (1.-GAM)*(1.-4.*GAM*ALFA/(1.-GAM)**2)**.5)/(2.*GAM*ALFA)      000201
00220 74*      PR=PP1*ALFA      000220
00221 75*      TTI = TEM+.5*PP1*(GAM*(PR*PR-1.)/(AM1+CPR(NPT)*PR))      000222
00222 76*      202 WRITE(JOUT,203) 11,PP1,TT1      000235
00230 77*      203 FORMAT(13,2E20.8)      000247
00231 78*      TPE = .TRUE.      000247
00232 79*      IT = TTI*(1)      000251

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00233 80* 205 ITR= ITR+1
00234 81* PP = PP1*P(IP)
00235 82* CALL EQLBPM
00236 83* IF (NPT.EQ.0) GO TO 1000
00240 84* IF (YT -LE- 0.0) GO TO 860
00242 85* GAM= GAMMA(NPT)
00243 86* RRI = PP1*WM(NPT)/AM1/TT1
00244 87* A11= 1./PP1 + 6AM*RRI*DLVPT(NPT)
00245 88* A12= GAM*RRI*DLVPT(NPT)
00246 89* A21= 5.6AM*(RRI**2-1.-DLVPT(NPT)*(1.+(RRI**2)))*DLVPT(NPT)-1.
00247 90* A22=-5.6AM*DLVPT(NPT)*(RRI**2-1.-WM(NPT)*CPR(NPT)
00250 91* B1= 1./PP1-1.6AM*(RRI-1.)
00251 92* B2= WM(NPT)*(HSM(NPT) - H1(NPT)/RRI)/TT - 0.5*6AM*(RRI**2 - 1.)
00252 93* X1 = XX(A22,B1,A12,B2,A11,A21)
00253 94* X2 = XX(A11,B1,A21,B1,A22,A12)
00254 95* ALAM= 1.
00255 96* TEM = X1
00256 97* IF (TEM.LT.0.) TEM = -TEM
00260 98* IF (X2.GT. TEM) TEM=X2
00262 99* IF (-X2.GT. TEM) TEM = -X2
00264 100* IF (TEM.GT. 0.) ALAM=-.N/TEM
00266 101* PP1= PP1*EXP(X1*ALAM)
00267 102* TT1= TT1*EXP(X2*ALAM)
00270 103* TT = TT1*TT1
00271 104* UD = RRI*SORT(RRI*GAM*TT/WM(NPT))
00272 105* WRITE(JOUT,30)ITR,PP1,TT1,RRI,X1,X2
00302 106* 30 FORMAT THCIER = ,I2,5X,6MP/P1 =,E15.8,5X,6MT/TT =,E15.8,5X,10MRHO/
00302 107* IPHO1 =,E15.8,7X,13HDEL LN P/P1 =,E15.8,5X,13HDEL LN T/TT =,E15.8)
00302 108* C CONVERGENCE TEST
00303 109* IF (ITR-LE-10 .AND. TEM.GT.0.5E-04) GO TO 205
00305 110* RRI0(NPT)=RRI
00306 111* IF (CP(NPT) -LE- 0.0) GO TO 40
00310 112* GM1(NPT) = CP(NPT)/(CP(NPT) - RRIAR/AM1)
00311 113* VMOC(NPT) = UD/SORT(RRI*GM1(NPT)*T(IT)/AM1)
00312 114* GO TO 150
00313 115* 40 GM1(NPT) = 0.
00314 116* VMOC(NPT) = 0.
00315 117* 150 K = 0
00316 118* IF (IP .EQ. NP .AND. IT .EQ. NT .OR. YT -LE- 0.0) GO TO 860
00320 119* K = NPT
00321 120* IF (NPT.NE.13) GO TO 870
00321 121* C OUTPUT
00323 122* 860 WRITE(JOUT,5)
00325 123* 5 FORMAT(1H1,2X,4HDETONATION PROPERTIES OF AN IDEAL REACTING GAS )
00326 124* CALL OUT1
00327 125* WRITE(JOUT,6)
00331 126* 46 FORMAT(13H UNBURNED GAS//)
00332 127* FMT(3) = F13
00333 128* FMT(4) = FOUR
00334 129* WRITE(JOUT,FMT) FP1,FR,FB,(PUB(J), J = 1,NPT)
00345 130* FMT(4) = TWO
00346 131* WRITE(JOUT,FMT) FT,FB,(TUB(J), J = 1,NPT)
00356 132* WRITE(JOUT,FMT) FH,FR,TH1(J), J = 1,NPT)
00360 133* DO 56 J = 1,NPT
00371 134* V(J) = AM1
00372 135* 56 SONVEL(J) = SORT(RRI*GM1(J)*TUB(J)/AM1)

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000374 130* FMT(4) = THREE
000375 131* WRITE(JOUT,FMT) FM,FB,(V(J), J = 1,NPT)
000376 132* FMT(4) = FOUR
000377 133* WRITE(JOUT,FMT) FCP,(CP(J), J = 1,NPT)
000378 134* WRITE(JOUT,FMT) FG,FB,FB,(CH(J), J = 1,NPT)
000379 135* FMT(4) = ONE
000380 136* WRITE(JOUT,FMT) FSV,FVEL,(SONVEL(J), J = 1,NPT)
000381 137* WRITE(JOUT,FMT)
000382 138* FMT(3) = ONE
000383 139* CALL OUT2
000384 140* WRITE(JOUT,68)
000385 141* 68 FORMAT(22H,DEFINITION PARAMETERS //)
000386 142* FMT(4) = THREE
000387 143* DO 70 J = 1,NPT
000388 144* V(J) = PPP(J)/PUB(J)
000389 145* PCP(J) = T1(J)/TUB(J)
000390 146* 70 SONVEL(J) = SONVEL(J)*RRHO(J)
000391 147* WRITE(JOUT,FMT) FPP,FB,FB,(V(J), J = 1,NPT)
000392 148* WRITE(JOUT,FMT) FTT,FB,FB,(PCP(J), J = 1,NPT)
000393 149* DO 73 J = 1,NPT
000394 150* V(J) = VM(J)/AM1
000395 151* FMT(4) = FOUR
000396 152* WRITE(JOUT,FMT) FNM,FB,FB,(V(J), J = 1,NPT)
000397 153* WRITE(JOUT,FMT) FRA,FB,FB,(RRHO(J), J = 1,NPT)
000398 154* WRITE(JOUT,FMT) FM,FB,(VMOC(J), J = 1,NPT)
000399 155* FMT(4) = ONE
000400 156* WRITE(JOUT,FMT) FUD,FVEL,(SONVEL(J), J = 1,NPT)
000401 157* EOL = TRUE
000402 158* CALL OUT3
000403 159* IF (K.EQ.0) AND. IOF .EQ. NOF) GO TO 1000
000404 160* IOF = IOF + 1
000405 161* WRITE(JOUT,868)
000406 162* 868 FORMAT(1H)
000407 163* NPT = 0
000408 164* 870 NPT = NPT + 1
000409 165* IF (K.EQ.1) K = -1
000410 166* CALL SAVE
000411 167* WRITE(JOUT,868)
000412 168* 902 CONTINUE
000413 169* IF (IOF.GE.NOF) GO TO 1000
000414 170* IOF = IOF + 1
000415 171* 1000 IF = .FALSE.
000416 172* RETURN
000417 173* END
000418 174*
000419 175*
000420 176*
000421 177*
000422 178*
000423 179*
000424 180*
000425 181*

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END OF COMPILATION:

ЭМРС.Р
ЕОЛБЭМ

AFOR, S EQLBPM, EQLBPM
HSA E3 -10/15/80-13:08:23 (16.)

SUBROUTINE EQLBPM ENTRY POINT 003120

STORAGE USED: CODE(1): 003136; DATA(0) 000461; BLANK COMMON(2) 000000

COMMON BLOCKS:

0003 CONSTS 000006
0004 HOLCON 000010
0005 POINTS 000335
0006 SPECES 017106
0007 MISC 001701
0010 DOUBLE 001560
0011 INDX 000041
0012 REF 000166
0013 CCC 000003

EXTERNAL REFERENCES (BLOCK, NAME)

0014 CP'S
0015 MAJORITY
0016 GAUSS
0017 ALOG
0020 MVDUS
0021 MIOIS
0022 MIOZS
0023 EXP
0024 MERR3S

STORAGE ASSIGNMENT (BLOCK, TYPE, RELATIVE LOCATION, NAME)

0001	001202	100L	0001	001211	101L	0001	002172	10276	0001	002222	1037G	0001	002213	110F
0001	001452	111L	0001	001575	1115L	0001	001633	1116L	0001	001517	113L	0001	002503	1134G
0001	001513	114L	0001	002511	1140G	0001	001542	115L	0001	002551	1154G	0001	001660	116L
0001	002624	1140L	0001	002454	1165L	0001	002716	1171L	0000	000214	1183F	0001	002644	1205G
0001	002676	1223G	0001	002741	1244G	0001	002046	13L	0001	001747	130L	0000	000321	136F
0001	002660	143L	0000	00257	144F	0001	002263	147L	0001	002270	148L	0001	000116	1516
0001	002516	153L	0001	002312	154L	0000	000265	156F	0001	002342	157L	0001	002401	158L
0001	002437	159L	0001	002152	160L	0000	000277	161F	0001	000151	1656	0001	002630	165L
0001	002450	166L	0000	000307	168F	0001	002616	169L	0001	002621	170L	0001	002725	171L
0000	000111	172F	0001	000430	174L	0001	0020G2	183L	0001	003013	186L	0000	000165	1924F
0001	00002	198L	0000	000326	201F	0001	001561	2115L	0001	000244	2216	0001	000277	232G
0000	000072	244F	0001	000325	245G	0001	000332	2516	0001	000374	2706	0001	000406	277G
0030	000220	306F	0001	000464	315G	0001	000512	3246	0001	000131	33L	0001	000613	360G
0000	000103	373F	0001	002653	40L	0001	000721	4166	0001	000732	4226	0001	000153	43L
0001	001003	445G	0001	001141	477G	0001	000125	499L	0001	001172	506G	0001	001252	531G
0001	001413	600G	0001	000213	62L	0001	000251	63L	0001	001444	631G	0001	000302	67L
0001	001625	673G	0001	001642	704G	0001	000342	72L	0001	001722	726G	0000	000107	73F
0000	000140	74F	0001	001760	746G	0000	000324	771F	0000	000075	772F	0001	000412	773L
0001	000524	77-L	0001	000536	775L	0000	000144	776F	0001	000747	80L	0001	000766	83L


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0001 001023 RNL 0001 001036 RSL 0001 000571 R71L 0001 003071 R73L 0001 000117 R74F
0001 001332 917L 0001 000146 923F 0001 000171 92AF 0001 000210 925F 0001 000603 968L
0001 000622 969L 0001 000632 969L 0001 001111 97L 0001 000635 970L 0001 000644 973L
0000 000232 973F 0000 000250 974F 0001 000654 997L 0006 R 000055 AMBDA1 0007 R 000705 AM1
0007 000150 ACAT 0007 000640 AM 0000 R 000054 AMBDA 0000 000000 ATMD 0007 R 000614 BQ
0007 001135 ANUM 0012 R 000133 APP 0003 000000 ATMN 0007 000000 ATCH 0007 R 000000 BQ
0007 000545 ROP 0011 000036 CALCH 0006 000000 COEF 0011 L 000001 CONVG 0005 R 000032 CPR
0007 000706 CPR2 0007 R 000634 CPSUM 0000 R 000040 CRITV 0007 000654 D2TA 0005 R 000067 DELF
0006 R 01424 DELN 0013 000002 DEMAND 0007 01560 DENS 0000 R 000053 DLNT 0005 R 000064 DLVPT
0005 R 000047 DLVTP 0006 000312 EN 0004 000000 ENO 0000 R 000037 ENL 0006 R 000045 ENSL
0007 001700 ENLSAV 0007 000000 ENN 0007 R 001676 ENNL 0000 001677 ENSAVE 0000 R 000057 FME51
0007 001414 ENTH 0012 000165 EOL 0007 R 001636 EGAT 0007 001445 FAZ 0000 R 000001 GAS
0007 000060 FNE62 0007 001527 FOX 0010 000000 G 0005 R 000101 GAMMAS 0004 000001 GAS
0003 000001 GMEY 0013 000000 GRAPH 0011 L 000003 HP 0007 000642 H PP 0007 000637 HSUBO
0005 R 000000 HSUM 0006 R 010376 HO 0000 I 000044 I 0011 L 000030 IC 0011 I 000000 IDEBUG
0004 I 000002 IE 0011 I 000015 IMAT 0000 I 000033 INC 0000 000421 IMJPS 0011 L 000023 IOMS
0011 000021 IP 0011 000037 IOSAVE 0011 I 000016 IOI 0000 I 00047 IOZ 0000 L 000034 ISING
0011 000003 ISV 0011 000034 II 0000 I 000042 ITUMB 0006 I 014244 IUSE 0004 000003 IZEPO
0000 I 000043 J 0000 I 000070 JOELF 0000 I 000051 JJ 0000 I 000065 JNG 0011 I 000026 JLIO
0013 I 000001 JOUT 0011 I 000025 JSOL 0011 I 000031 JS 0000 I 000064 K6 0011 I 000014 KMAT
0011 I 000012 L 0004 00004 LANK 0007 I 000463 LLMT 0000 L 00035 LOGV 0011 000040 LSAVE
0004 000005 MOL 0011 000035 MLES 0007 000707 NAME 0011 I 000024 NC 0000 I 000052 MEN
0011 000022 MEPR 0011 000035 MFZ 0011 000017 MOF 0011 000020 MOMIT 0011 000007 NP
0011 I 000011 NPT 0011 000027 MREAC 0011 I 000013 NS 0000 I 000000 NSPP1 0011 000010 NT
0000 I 000050 NTCRO 0000 I 000046 NUMB 0007 000635 OF 0004 000006 OX 0007 R 001644 OXF
0005 000116 P 0003 000002 PATH 0012 000000 PCP 0007 002363 PECMT 0007 R 000633 PP
0005 R 000217 PPP 0000 R 000001 PROM 0003 000003 PRAR 0003 000004 PRR 0007 000644 RH
0007 001611 RHOP 0000 L 000036 RTE 0007 001612 RMW 0007 001876 RTEMP 0003 R 000005 RVR
0006 R 004064 S 0011 L 000033 SHOCK 0000 R 000041 SIZEF 0006 016660 SLN 0005 000251 SONVEL
0011 L 000004 SP 0012 000047 SPIM 0000 R 000062 SS 0005 R 000015 SSUM 0006 R 012564 SUB
0012 000101 SUBAR 0000 000032 SUM 0007 R 000001 SUMN 0000 R 000056 SUM1 0012 000116 SUPAR
0007 R 000003 SO 0005 R 000150 T 0006 R 016514 TEMP 0007 R 000632 TMIGH 0007 R 001643 TLM
0007 R 000630 TLOW 0007 R 000627 TM 0000 R 000066 TMELT 0007 000631 TMID 0000 R 000071 TN
0005 R 000320 TOTN 0011 L 000002 TP 0007 R 000002 TT 0005 R 000266 TTT 0005 000202 V
0012 000064 VACT 0005 000030 VLM 0007 000646 VMIN 0012 000032 VMOC 0011 L 000032 VOL
0007 000650 VPLS 0005 R 000234 VM 0007 000652 WP 0010 001510 X 0004 000007 ZERO

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00101 1* SUBROUTINE EQLBRM 000000
00101 2* C 000000
00101 3* C ROUTINE TO CALCULATE EQUILIBRIUM COMPOSITION AND PROPERTIES 000000
00101 4* C 000000
00101 5* COMMON /ROWS C, ATMN, GMEY, PATH, RBAR, RBR, RVR 000000
00101 6* COMMON /HCO2CONZ ENO, GAS, IE, IZER, LANK, MOL, OX, ZERO 000000
00101 7* COMMON /POINTS/HSUM(13), SSUM(13), CPR(13), DLVTP(13), DLVPT(13) 000000
00101 8* 1, GAMMAS(13), P(26), T(26), X(13), PPR(13), WM(13), SONVEL(13), TTT(13) 000000
00101 9* 2, VLM(13), TOTN(13) 000000
00101 10* C COMMON/SPECES/COEF(2,7,150), S(150), EN(150,13), ENLW(150), HO(150) 000000
00101 11* C 1, DELN(150), A(15,150), SUB(150,3), IUSE(150), TEMPI(50,2), SLN(150) 000000
00101 12* INCLUDE SPECPR 000000
00101 13* COMMON /MISC/ EYN, SUMN, TT, SO, ATOM(3,101), LLMT(25), BO(25), 000000
00101 14* BOPI(25,2), TM, TLOW, TMID, THIGH, PP, CPSUM, OF, EGAT, 000000
00101 15* HSUBO, AM(2), HPP(2), PH(2), VMIN(2), VPLS(2), WP(2), 000000
00101 16* DATA(25), AM1, CPPI, NAME(25,6), ANUM(25,6), PECMT(25), 000000

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00112 17* ENTH(25),FAZ(25),RTEMP(25),FOX(25),DEN(25),RHOP,
00113 18* RHV(25),VLN,OXF(26),ENNL,ENSAVE,ENLSA
00114 19* COMMON /DOUBLE/ G(20,21),X(20)
00115 20* COMMON /INDEX/ IDEBUG,CONVG,TP,MP,SP,TSV,MOLES,MP,NT,NPT,L,MS,
00116 21* KMAT,I,MAT,IQI,NOF,NOMIT,IP,NEUR,IONS,NC,JSOL,JLIQ,
00117 22* HREAC,IC,J51,YDL,SHOCK,IT,MFZ,CALCM,IQSAVE,LGAVE,
00118 23* COMMON /PERF/ PCP(26),VMOC(13),SPIM(13),VACI(13),SUBAR(13),
00119 24* SUPAR(13),APPI(13),AEAT(13),EQL
00120 25* COMMON /CCC/ GRAPH,JOUT,DEMAND
00121 26* COMMON /PRECISION G,SUM,X
00122 27* LOGICAL CONVG,MP,IC,IONS,ISING,LOGY,RITE,SHOCK,SP,TP,VOL
00123 28* DIMENSION PROM(25)
00124 29* DOUBLE PRECISION G,SUM,X
00125 30* LOGICAL CONVG,MP,IC,IONS,ISING,LOGY,RITE,SHOCK,SP,TP,VOL
00126 31* ENL = ENNL
00127 32* RITE = .FALSE.
00128 33* IF(IDEBUG,GT,0,AND,NPT,GE,IDEBUG) RITE=.TRUE.
00129 34* CRITV = 5.0E-6
00130 35* SIZEF = 0.
00131 36* ISING = .FALSE.
00132 37* LOGV = .FALSE.
00133 38* IF (VOL) PP = RVR*ENNT/VLM(NPT)
00134 39* TUN = ALOG(11)
00135 40* CONVG = .FALSE.
00136 41* ITNUMB = 100
00137 42* JS1 = 1
00138 43* CALL CPHS
00139 44* TM = ALOG(PP/ENM)
00140 45* IF(ICI) PREVIOUS POINT HAD SINGULAR MATRIX
00141 46* IF(ICI) GO TO 966
00142 47* IF (.NOT.IONS.OR.IE.EQ.LLMT(L)) GO TO 33
00143 48* L = L+1
00144 49* IQI = IQI+1
00145 50* DO 499 J = 1,MS
00146 51* IF (A(L,J).EQ.0.) GO TO 499
00147 52* ENL(J,MPT) = 1-E-8
00148 53* ENL(J) = -18.4706810
00149 54* IUSE(J) = 0
00150 55* 499 CONTINUE
00151 56* 33 IF(NPT,EQ,1,AND,.NOT. SHOCK) WRITE(JOUT,244)(LLMT(I),I=1,L)
00152 57* 244 FORMAT(1HPT,14(SX,AN))
00153 58* BEGIN ITERATION
00154 59* 43 IF(ICI) GO TO 1171
00155 60* IF (.NOT.CONVG) GO TO 62
00156 61* SUM = ENL
00157 62* IF(JSOL.EQ.0) GO TO 62
00158 63* ENSOL = EN(JSOL,MPT)
00159 64* ENL(JSOL,MPT) = EN(JSOL,MPT)+EN(JLIQ,MPT)
00160 65* IUSE(JLIQ) = -IUSE(JLIQ)
00161 66* IQI = IQI-1
00162 67* DLT(NPT) = 0.
00163 68* CPR(MPT) = 0.
00164 69* GAMMA(SINPT) = 0.
00165 70* LOGV = .TRUE.
00166 71* 62 CALL MATRIX
00167 72*

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0212 730 NOMP = 101 - ITNUMB 000214
0213 740 I02 = I01 + 1 000217
0214 750 IF (.NOT. CONVS) GO TO 67 000222
0215 760 IF (LOGV.AND.(J01.EQ.0)) GO TO 63 000224
0216 770 DO 102 I=1,L 000224
0217 780 102 PROMI = G(I01,I) 000224
0218 790 IF (.NOT. LOGV) GO TO 67 000226
0219 800 LOGV = .TRUE. -- SET UP MATRIX TO SOLVE FOR DLVPT 000226
0220 810 63 G(I01,I02) = ENM 000251
0221 820 J = I01 - 1 000260
0222 830 DO 775 I = 1,J 000270
0223 840 775 G(I,I02) = G(I,I01) 000277
0224 850 67 IF (.NOT.RITE) GO TO 72 000302
0225 860 WRITE(JOUT,772) NUMB 000303
0226 870 772 FORMAT (11M01TERATION ,I3,6X,7MMATRIX //) 000325
0227 880 DO 911 I=1,IMAT 000325
0228 890 911 WRITE(JOUT,73) (G(I,J), J = 1,IMAT) 000325
0229 900 72 IF (CONVE) IMAT=IMAT-1 000342
0230 910 J = IMAT 000346
0231 920 CALL GAUSS 000350
0232 930 IF (J.NE. IMAT) GO TO 774 000352
0233 940 IF (.NOT.RITE) GO TO 773 000355
0234 950 WRITE(JOUT,773) (LMT(I),I=1,L) 000363
0235 960 773 FORMAT (7M01,1X,17(A9,10X)) 000377
0236 970 WRITE(JOUT,73) (X(I),I=1,IMAT) 000412
0237 980 73 FORMAT (9E10,6) 000412
0238 990 773 IF (.NOT. CONVG) GO TO 85 000413
0239 1000 IF (.NOT. LOGV) GO TO 174 000421
0240 1010 IF (LOGV.NE.0) ENUSOL,MPTI=ENSOL 000424
0241 1020 GO TO 171 000426
0242 1030 174 SUM = 0. 000430
0243 1040 DO 175 J=1,L 000431
0244 1050 175 SUM = SUM + PROMI(J)*X(J) 000464
0245 1060 DLVPT(MPT) = 1.+G(I02,I01)/ENM-SUM/ENM - X(I01) 000470
0246 1070 CPMPTI = G(I02,I02) 000502
0247 1080 DO 176 J=1,I01 000512
0248 1090 176 CPMPTI = CPMPTI - G(I02,J)*X(J) 000512
0249 1100 LOGV = .TRUE. 000520
0250 1110 GO TO 62 000522
0251 1120 C SINGULAR MATRIX 000524
0252 1130 774 IF (.NOT. CONVG) GO TO 775 000524
0253 1140 C IF (ISING) SINGULAR OMCE 000524
0254 1150 C IF (IC) SINGULAR TWICE 000524
0255 1160 WRITE(JOUT,172) 000524
0256 1170 172 FORMAT(28HDERIVATIVE MATRIX SINGULAR ) 000532
0257 1180 IC = .TRUE. 000532
0258 1190 GO TO 171 000534
0259 1200 775 IF (.NOT. MP.GP.MPTI.NE.1.OR.MC.EQ.0.OR.TT.GT.100.) GO TO 871 000536
0260 1210 WRITE(JOUT,874) 000562
0261 1220 874 FORMAT(96HLOW TEMPERATURE IMPLIES CONDENSED SPECIES SHOULD HAVE 000567
0262 1230 BEEN INCLUDED ON AN INSERT CARD, RESTART ) 000567
0263 1240 GO TO 873 000571
0264 1250 871 WRITE(JOUT,74) 000571
0265 1260 74 FORMAT(16HSINGULAR MATRIX) 000575
0266 1270 IF (IC) GO TO 873 000575
0267 1280 IF (ISING) GO TO 957 000577

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00505 185*      DO 99 I = 1,L
00510 186*      DELN(I) = DELN(J) + A(I,J)*X(I)
00512 187*      GO TO 101
00513 190*      100 DELN(I) = X(I,J)
00514 189*      JJ = JJ + 1
00515 190*      101 CONTINUE
00517 191*      AMBDA = 1.
00520 192*      SUM = X(I,J)
00521 193*      IF (SUM,LT,0.) SUM = -SUM
00522 194*      IF (SUM,GT,0.) SUM = SUM
00523 195*      IF (SUM,GT,0.) SUM = DLNT
00526 196*      IF (SUM,GT,0.) SUM = -DLNT
00530 197*      DO 917 J=1,NS
00533 198*      IF (IUSE(J),NE,0.) GO TO 917
00535 199*      IF (IEN(J,NPT) .GT. 0.0 .AND. DELN(J) .GT. SUM) SUM = DELN(J)
00537 200*      IF (IEN(J,NPT) .GT. 0.0 .OR. DELN(J) .LE. 0.0) GO TO 917
00541 201*      SUM1 = (-9.212-ENLN(J) + ENL)/(DELN(J)-X(I,J))
00542 202*      IF (SUM1,LT,0.) SUM1 = -SUM1
00544 203*      IF (SUM1,LT,AMBDA) AMBDA1 = SUM1
00546 204*      917 CONTINUE
00550 205*      IF (SUM,GT,2.) AMBDA = 2./SUM
00552 206*      IF (AMBDA1,LT,AMBDA) AMBDA = AMBDA1
00554 207*      IF (NOT,RITE) GO TO 111
00556 208*      WRITE(JOUT,923) I,ENL,ENL,PP,IM,AMBDA
00566 209*      923 FORMAT (3HGT=E15.8,6H ENL=E15.8,7H ENML=E15.8,5H PP=E15.8,
00567 210*      1 9H LN P/N=E15.8,8H AMBDA=E15.8)
00573 211*      IF (VOL) WRITE(JOUT,924) VLM(NPT)
00574 212*      1924 FORMAT (8H VOLUME=E15.8,2HCC)
00576 213*      WRITE(JOUT,924)
00577 214*      924 FORMAT (1H0,18X,2HMT,12X,5HLM N1,8X,9HDEL LM N1,10X,4HMT/RT,9X,4HSD/
00578 215*      RT,12X,6H-60/RT,9X,5H-6/RT)
00579 216*      DO 926 J=1,NS
00602 217*      FNEG1 = S(IJ)-HQ(J)
00603 218*      FNEG2 = FNEG1
00604 219*      IF (IUSE(J),EQ,0) FNEG2 = FNEG2-ENLN(J)-IM
00606 220*      926 WRITE(JOUT,925) SUB(J,1),SUB(J,2),SUB(J,3),EN(J,NPT),ENLN(J),
00607 221*      DELN(J),HQ(J),S(IJ),FNEG1,FNEG2
00623 222*      925 FORMAT (1X,3AN,7E15.6)
00624 223*      WRITE(JOUT,110)
00626 224*      110 FORMAT (1H0)
00627 225*      C APPLY CORRECTIONS TO ESTIMATES
00628 226*      111 SUM = 0.
00630 227*      DO 113 J=1,NS
00633 228*      IF (IUSE(J)) 113,112,114
00636 229*      112 ENLN(J) = ENLN(J) + AMBDA*DELN(J)
00637 230*      EN(J,NPT) = 0.
00640 231*      IF (ENLN(J) + 19.4206810 .LE. ENL) GO TO 113
00642 232*      EN(J,NPT) = EXP(ENLN(J))
00643 233*      SUM = SUM + EN(J,NPT)
00644 234*      GO TO 113
00645 235*      114 EN(J,NPT) = EN(J,NPT) + AMBDA * DFLN(J)
00646 236*      113 CONTINUE
00650 237*      SUMN = SUM
00651 238*      IF (TP) GO TO 115
00653 239*      TLM = TLM + AMBDA*DLNT
00654 240*      T = EXP(TLM)

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00655 2410 JS1 = 1
00656 2420 CALL CPMS
00657 2430 115 IF (VOL) GO TO 2115
00661 2440 ENL = ENL+AMDA*X(IQ1)
00662 2450 ENL = EXP(ENL)
00663 2460 GO TO 1115
00664 2470 2115 ENL = SUM
00665 2480 ENL = ALOG(ENL)
00666 2490 PP = RVR*TT*ENL/VLM(NPT)
00667 2500 1115 TM = ALOG(PP/ENL)
00670 2510 IF (LMT(L).NE.IE) GO TO 116
00670 2520 C CHECK ON REMOVING IONS
00672 2530 DO 1116 J = 1,NS
00675 2540 IF (AIL(J).EQ.0.1) GO TO 1116
00677 2550 IF (ENIJ.NPT).GT.0.1) GO TO 116
00701 2560 1116 CONTINUE
00703 2570 DO 1118 J=1,NS
00706 2580 1118 IF (AIL(J).NE.0.0) IUSE(IJ) = 10000
00711 2590 L = L-1
00712 2600 IQ1 = IQ1-1
00713 2610 GO TO 43
00713 2610 C TEST FOR CONVERGENCE
00713 2620 IF (ITNUMB.EQ.0) GO TO 13
00714 2630 116 IF (AMDA.LT.1.1) GO TO 43
00716 2640 SUM = (ENL-SUM)/ENL
00720 2650 IF (SUM.LT.0.1) SUM = -SUM
00721 2660 IF (SUM.GT.0.1) GO TO 43
00723 2670 DO 130 J=1,NS
00725 2680 IF (IUSE(J).LT.0.1) GO TO 130
00730 2690 AA = DELN(J)/SUM
00732 2700 IF (AA.LT.0.1) AA = -AA
00733 2710 IF (IUSE(J).EQ.0) AA = AA*EN(J,NPT)
00735 2720 IF (IAA.GT.0.1) GO TO 43
00737 2730 130 CONTINUE
00741 2740 C CALCULATE ENTROPY, CHECK ON DELTA S FOR SP PROBLEMS
00741 2750 TOTM(NPT) = 0.
00743 2760 SSUM(NPT) = 0.
00744 2770 DO 183 J=1,NS
00745 2780 IF (IUSE(J).LT.0.1) GO TO 183
00750 2790 TOTM(NPT) = TOTM(NPT) + EN(J,NPT)
00752 2800 SS = SS(J)
00753 2810 IF (IUSE(J).EQ.0) SS = SS-ENM(J)-TM
00754 2820 SSUM(NPT) = SSUM(NPT) + SS*EN(J,NPT)
00756 2830 183 CONTINUE
00757 2840 IF (.NOT.SP.OR.NPT.EQ.1) GO TO 13
00761 2850 SS = SSUM(NPT) - SO
00763 2860 IF (SS.LT.(-0.00005).OR.SS.GT.0.00005) GO TO 43
00764 2870 IF (RITE) WRITE(JOUT,1183) SS
00766 2880 1183 FORMAT(12HDELTA S/R =,E15.8)
00772 2890 13 CONVE = .TRUE.
00773 2900 IF (ITLW.OR.TT) .GT.THIGHWRITE(JOUT,306)TT,NPT
00774 2910 306 FORMAT(17HTHE TEMPERATURE=E12.4,26H IS OUT OF RANGE FOR POINT,15)EOLM0119
00774 2920 IF (ITNUMB.NE.0) GO TO 160
00774 2930 WRITE(JOUT,973) NPT
00774 2940 973 FORMAT (175H,69H100 ITERATIONS DID NOT SATISFY THE CONVERGENCE REQ
00774 2950 1183 HMENTS FOR POINT,13/)
00774 2960

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01010 297*      WRITE (JOUT,974) TT
01013 298*      974 FORMAT (5X,'#### TEMPERATURE=',F12.0,' 0000')
01014 299*      IF (.NOT. MP.OR. NPT.NE.1.OR. NC.EQ.0.OR. TT.GT.100.) GO TO 873
01016 300*      WRITE (JOUT,874)
01017 301*      TT = T(1)
01021 302*      RETURN
01021 303*      C CONVERGENCE TESTS ARE SATISFIED, TEST CONDENSED SPECIES.
01022 304*      160 IF (NC.EQ.0) GO TO 143
01024 305*      SIZEF = 0.
01025 306*      INC = 0
01026 307*      DO 170 J = 1, NS
01031 308*      IF (IUSE(J).EQ.0 .OR. IUSE(J).EQ.-100001) GO TO 170
01033 309*      INC = INC + 1
01034 310*      IF (RITE) WRITE (JOUT,144) (SUB(J,I), I=1,3), TEMP(INC,1), TEMP(INC,2),
01034 311*      IUSE(J), EN(J,NPT)
01034 312*      144 FORMAT (10H,3A4,2F10.3,3X,5HIUSE=,I4,E15.7)
01050 313*      IF (EN(J,NPT)) 146,148,149
01053 314*      146 IF (JANE.JSOL.AND. J.NE.JL10) GO TO 147
01055 315*      JSOL = 0
01056 316*      JL10 = 0
01057 317*      147 IQ1 = IQ1 - 1
01060 318*      EN(J,NPT) = 0.
01061 319*      GO TO 166
01062 320*      148 MG = 1
01063 321*      IF (IUSE(J).EQ.-IUSE(J+1)) GO TO 154
01065 322*      IF (J.EQ.1 .OR. IUSE(J).NE. -IUSE(J-1)) GO TO 153
01067 323*      MG = -1
01070 324*      154 JMG = J + MG
01071 325*      IF (EN(JMG,NPT).LT.0.) GO TO 170
01073 326*      TMELT = TEMP(INC,1)
01074 327*      IF (TMELT.EQ. TEMP(INC+MG,2)) GO TO 158
01076 328*      TMELT = TEMP(INC,2)
01077 329*      IF (TMELT.EQ. TEMP(INC+MG,1)) GO TO 157
01101 330*      WRITE (JOUT,156)
01103 331*      156 FORMAT (50H,3 PHASES OF A CONDENSED SPECIES ARE OUT OF ORDER )
01103 332*      C JTH SPECIES A SOLID (EN=0), J*MGJTH SPECIES A LIQUID (EN.IS.1)
01104 333*      157 IF (TT.GT. TMELT .OR. (TP.AND. TT.EQ. TMELT)) GO TO 169
01106 334*      IF (TP .OR. TT.LE. TMELT - 150.0) GO TO 1165
01110 335*      JSOL = J
01111 336*      JL10 = JMG
01112 337*      GO TO 159
01112 338*      C JTH SPECIES A LIQUID (EN=0), J*MGJTH SPECIES A SOLID (EN IS.1)
01113 339*      158 IF (TT.LT. TMELT .OR. (TP.AND. TT.EQ. TMELT)) GO TO 169
01115 340*      IF (TP .OR. TT.GE. TMELT + 150.0) GO TO 1165
01117 341*      JSOL = JMG
01120 342*      JL10 = J
01121 343*      159 TLM = ALOG (TMELT)
01122 344*      TT = TMELT
01123 345*      EN(JMG,NPT) = .5 * EN(JMG,NPT)
01124 346*      EN(J,NPT) = EN(JMG,NPT)
01125 347*      GO TO 165
01125 348*      C WRONG PHASE INCLUDED FOR T INTERVAL, SWITCH FN
01126 349*      1165 EN(J,NPT) = EN (JMG, NPT)
01127 350*      IUSE(J) = -IUSE(J)
01130 351*      IUSE (JMG) = -IUSE(JMG)
01131 352*      EN(JMG,NPT) = 0.

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01132 3530 WRITE(JOUT,16) (SUB(JG,1), I = 1,3), (SUB(J,1), I = 1,3) 002471
01144 3540 161 FORMAT (10X,22PHASE CHANGE, REPLACE ,3A,6M WITH ,3A) 002514
01145 3550 GO TO 40 002514
01146 3560 153 IF (TT-LI-TEMP(INC,1) -AND-TEMP(INC,1) NE,TLOW) GO TO 169 002516
01150 3570 IF (TT-GT-TEMP(INC,2)) GO TO 169 002533
01152 3580 SUM = 0. 002492
01153 3590 DO 167 I = 1,L 002551
01156 3600 167 SUM = SUM + A(I,J)*X(I) 002551
01160 3610 DELF = HO(I)-S(J)-SUM 002555
01161 3620 IF(ITE) WRITE(JOUT,16)IDELF,SIZEF 002563
01166 3630 168 FORMAT (17H GO-SUM(AI,JP1) =E15.7,10X,18PREVIOUS DELTA 6 =,E15.7) 002574
01167 3640 IF(IDELF,GE,SIZEF) OR, DELF,GE,0.1 GO TO 169 002574
01171 3650 SIZEF = DELF 002611
01172 3660 IDELF = J 002613
01173 3670 169 IF(INC-EQ,NC) GO TO 1160 002616
01175 3680 170 CONTINUE 002624
01177 3690 1160 IF (SIZEF-EQ,0.) GO TO 143 002624
01201 3700 J = JDELF 002628
01202 3710 165 IQ1 = IQ1 + 1 002630
01203 3720 WRITE(JOUT,136) (SUB(J,1), I = 1,3) 002632
01211 3730 136 FORMAT (10X,9HADD ,3A) 002650
01212 3740 166 IUSE(J) = - IUSE(J) 002650
01213 3750 40 CONVG = .FALSE. 002653
01214 3760 JSA = 1 002653
01215 3770 CALL CPHS 002655
01216 3780 143 TN = NUMB 002660
01217 3790 IF (.NOT. SHOCK) WRITE(JOUT,771) NPT,X(I), I = 1,L),TN 002662
01230 3800 771 FORMAT (13,14F9.3) 002703
01231 3810 JSA = 1 002703
01232 3820 IF(ITP,AND,CONVG) CALL CPHS 002705
01234 3830 ITNUMB = 100 002712
01235 3840 GO TO 43 002714
01235 3850 C CALCULATE EQUILIBRIUM PROPERTIES 002714
01236 3860 1171 DLVPT(NPT) = -1. 002716
01237 3870 DLVPT(NPT) = 1. 002720
01240 3880 CPR(NPT) = CPSUM 002721
01241 3890 GO TO 199 002723
01242 3900 171 SUM = 0. 002725
01243 3910 DO 179 J = 1,L 002726
01246 3920 179 SUM = SUM + PROM(J)*X(J) 002741
01250 3930 DLVPT(NPT) = -2.*SUM/ENN + X(I01) 002745
01251 3940 IF (JLIQ -EQ, 0) GO TO 199 002754
01253 3950 IUSE(JLIQ) = -IUSE(JLIQ) 002756
01254 3960 HSUM(NPT) = HSUM(NPT)*EN(JLIQ,NPT)*(HO(JLIQ)-HO(JSOL)) 002761
01255 3970 IQ1 = IQ1+1 002772
01256 3980 GAMMAS(NPT) = -1./DLVPT(NPT) 002775
01257 3990 GO TO 186 003000
01260 4000 199 GAMMAS(NPT) = -1./DLVPT(NPT)*(DLVPT(NPT)+2)*ENN/CPR(NPT) 003002
01261 4010 186 TT(NPT) = TT 003013
01262 4020 ENNL = ENL 003015
01263 4030 PPP(NPT) = PP 003017
01264 4040 VLM(NPT) = RVR*ENN*TT/PP 003021
01265 4050 HSUM(NPT) = HSUM(NPT)*TT 003026
01266 4060 WH(NPT) = 1./ENN 003031
01267 4070 IF (.NOT. RTE) RETURN 003035
01271 4080 WRITE(JOUT,201) NPT,APP(NPT),PP,TT,HSUM(NPT),SSUM(NPT),WM(NPT), 003042
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OF POOR QUALITY

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01271 409* 1 CPRI(MPT),OLVPT(MPT),OLVTP(MPT),GAMMAS(MPT),VL(MMPT)
01307 410* 201 FORMAT (7HOPOINT=I3.6,3X,4HPCP=E13.6,3X,2HP=E13.6,3X,MT=E13.6,3X,4M
01307 411* 1M/R=E13.6,3X,4MS/R=E13.6//3X,3MM=E13.6,3X,5HCP/R=E13.6,3X,6HOLVPT
01307 412* 2=E13.6,3X,6HOLVTP=E13.6,3X,9H6AMMAIS=E13.6,3X,2H4=E13.6)
01310 413* RETURN
01310 414* C ERROR. SET TT=0
01311 415* 873 TT=0
01312 416* MPT = MPT-1
01313 417* RETURN
01314 418* END

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END OF COMPILATION: NO DIAGNOSTICS.

END6.P FROZEN

FROZEN

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FOR.S FROZEN,FROZEN
MSA E, -10/16/80-13:06:33 (10.)

SUBROUTINE FROZEN ENTRY POINT 000395

STORAGE USED: CODE(1) 000360: DATA(0) 000041: BLANK COMMON(2) 000000

COMMON BLOCKS:

0003 CONSIS 000006
0004 POINTS 000335
0005 SPECES 017104
0006 MISC 001701
0007 INDX 000041

EXTERNAL REFERENCES (BLOCK, NAME)

0010 PMS
0011 ALOG
0012 EXP
0013 MERR35

STORAGE ASSIGNMENT (BLOCK, TYPE, RELATIVE LOCATION, NAME)

0001	000066	1356	0001	000251	2076	0001	000022	51L	0001	000350	55L	0001	000120	60L												
0001	000145	AIL	0001	000111	901L	0001	000321	903L	0005	011052	A	0004	000490	AM												
0006	000705	AM1	0006	001135	ANUM	0003	000000	ATM	0006	000009	ATOM	0006	000519	BD												
0006	000545	BOP	0007	000036	CALCH	0000	000005	CC	0005	000000	COEF	0007	L	000001	CONVG											
0004	R	000032	CPR	000706	CPR1	0006	R	000639	CPSUM	0006	000659	DATA	0005	010424	OELM											
0006	001560	DENS	0000	R	000007	DLMT	0004	R	000064	DLVPT	0004	R	000047	DLVTP	0005	R	000312	EN								
0005	010150	ENLM	0006	001700	ENLSAV	0006	G	000000	ENM	0006	001676	ENML	0006	001677	ENSAVE	0004	R	000101	BARRAS							
0006	001319	ENTM	0006	000434	EGRAT	0006	001335	FAZ	0006	000642	HPP	0006	R	000000	MSUM	0004	R	000000	MSUM							
0003	000001	GMEY	0007	L	000003	HP	0006	000642	HPP	0007	000015	IMAT	0000	I	000010	INC	0000	I	000010	INC						
0005	R	010376	MO	0007	000030	IC	0007	000000	IDEBUS	0007	000021	IP	0007	000016	IQ	0007	000026	JL10	0007	000040	LSAVE					
0000	000015	INJPS	0007	000023	IONS	0007	000021	IP	0005	I	016266	IUSE	0006	000643	LLMT	0007	000035	MF2	0007	I	000011	MPT				
0007	000005	ISV	0007	000039	IT	0005	I	016266	IUSE	0006	000643	LLMT	0007	000022	MEVR	0007	I	000011	MPT	0007	I	000011	MPT			
0007	000025	J50L	0007	I	000031	J51	0007	000014	KMAT	0007	000022	MEVR	0007	I	000011	MPT	0007	I	000011	MPT	0007	I	000011	MPT		
0007	000004	MOLES	0006	000707	NAME	0007	I	000024	MC	0007	000007	NP	0007	I	000011	MPT	0007	I	000011	MPT	0007	I	000011	MPT		
0007	000012	NLM	0007	000017	NOF	0007	000020	NOFIT	0007	000010	NT	0006	000635	OF	0006	R	000633	PP	0006	R	000633	PP	0006	R	000633	PP
0007	000027	NREAC	0007	I	000013	NS	0000	I	000000	MSPP1	0006	001363	PECUT	0006	R	000633	PP	0006	R	000633	PP	0006	R	000633	PP	
0006	001649	OXF	0004	000116	P	0003	000002	PATM	0006	000649	RM	0006	001611	RMOP	0006	R	000633	PP	0006	R	000633	PP	0006	R	000633	PP
0004	R	000217	PPP	0003	000003	RRAR	0003	000004	RBR	0003	R	000005	RVR	0005	R	000644	S	0005	R	000644	S	0005	R	000644	S	
0006	001612	RMV	0000	R	000001	RMV	0006	001612	RMV	0007	L	000004	SP	0000	R	000006	SS	0000	R	000006	SS	0000	R	000006	SS	
0007	000033	SMOCH	0005	016660	SLM	0004	QQ251	SONVEL	0004	QQ251	SONVEL	0004	QQ251	SONVEL	0004	QQ251	SONVEL	0004	QQ251	SONVEL	0004	QQ251	SONVEL	0004	QQ251	SONVEL
0004	R	000015	SSUM	0005	015364	SUB	0000	R	000003	SUMH	0004	000001	SUMH	0004	000001	SUMH	0004	000001	SUMH	0004	000001	SUMH	0004	000001	SUMH	
0006	R	000003	SO	0004	000150	T	0005	R	016514	TEMP	0006	000632	THIGH	0006	R	000632	THIGH	0006	R	000632	THIGH	0006	R	000632	THIGH	
0006	R	000030	TLOW	0006	000627	TM	0006	000631	TMID	0004	R	000320	TOTM	0007	000002	TP	0007	000002	TP	0007	000002	TP	0007	000002	TP	
0006	R	000002	TY	0004	R	000266	TYT	0004	000202	V	0004	R	000303	VLM	0006	R	000646	VMIN	0006	R	000646	VMIN	0006	R	000646	VMIN
0007	L	000032	VOL	0006	000650	VPLS	0004	R	000239	WM	0006	000652	WP	0006	R	000652	WP	0006	R	000652	WP	0006	R	000652	WP	

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00101 1* SUBROUTINE FROZEN
00101 2*
00101 3* C (FROZEN COMPOSITION EXPANSION ONLY)
00101 4* C
00101 5* COMMON /CONST/ ATOM, CHEI, PAIR, RBAR, RBR, RVR
00101 6* COMMON/POINTS/ MSUM(13), SSUM(13), CPR(13), DLVPT(13), DLVPT(13)
00101 7* 1 .GAMMA(13), P(26), V(13), PPP(13), MM(13), SONVEL(13), TTT(13)
00101 8* 2 .VLM(13), TOTM(13)
00101 9* COMMON/SPECIES/ COEF(2,7,150), S(150), ENL(150,13), ENLM(150), W(150)
00101 10* 1 .DELTM(150), A(15,150), SUB(150,3), IUSE(150), TEMP(SQ,2), SLN(150)
00101 11* INCLUDE SPECPA
00101 12* COMMON /MISC/ ENM, SUM, TT, SO, ATOM(3,101), LLMT(25), BO(25),
00101 13* BOP(25,2), TM, TLOW, TMID, THIGH, PP, C, SUM, OP, EQRAY,
00101 14* HSUBO, AM(2), HPP(2), RM(2), VM(2), VMIN(2), NPLS(2), UP(2),
00101 15* DATA(25), AM1, CPRI, NAME(25,6), ANUM(25,6), PECWT(25),
00101 16* ENTH(25), FAZ(25), RTEMP(25), FOX(25), DEN(25), RHOP,
00101 17* RHV(25), XLM, QRE(26), ENML, ENSAVE, ENLSAV
00101 18* COMMON /IMDX/ IDEBUG, CONVG, TP, MP, SP, ISV, MOLES, MP, MT, NPT, NLM, MS,
00101 19* RMAT, IMA, IOI, MOI, NOMI, IP, NEWP, IONS, MC, JSOL, JULIO,
00101 20* NREAC, IC, JSI, VOL, SMOCK, IT, NFZ, CALCH, IOSAVE, LSAVE
00101 21* C
00101 22* LOGICAL CONVG, MP, SP, VOL
00101 23* C
00101 24* CONVG = .FALSE.
00101 25* TLM = ALOG(TT)
00101 26* IF (VOL) RNV = RVR/(VLM(NPT)*WM(NFZ))
00101 27* S1 SUMS=0.
00101 28* SUMH = 0.
00101 29* JSI = 1
00101 30* J = NPT
00101 31* NPT = NFZ
00101 32* CALL CPMS
00101 33* CC = CPSUM
00101 34* IF (.NOT. VOL) 60 TO 55
00101 35* CC = CPSUM-1./WM(NFZ)
00101 36* PP = RNV*TT
00101 37* SS NPT = J
00101 38* DO 60 J = 1, MS
00101 39* IF (ENI(J, NFZ)) .LE. 0.0) 60 TO 60
00101 40* SS = S1(J)
00101 41* IF (IUSE(J, EQ, 0)) SS = SS - ALOG(EN(J, NFZ)) * PP * WM(NFZ)
00101 42* SUMS = SUMS + SS * EN(J, NFZ)
00101 43* IF (CONVG, OR, MP) SUMH = SUMH + HCL(J) * EN(J, NFZ)
00101 44* 60 CONTINUE
00101 45* IF (CONVG) 60 TO 81
00101 46* IF (SP) DLNT = (SUMS - S0)/CC
00101 47* IF (MP) DLNT = (SUMH - HSUBO/TT)/CC
00101 48* TLM = TLM - DLNT
00101 49* IF (DLNT, LT, 0.) DLNT = -DLNT
00101 50* IF (DLNT, LT, 0.5E-4) CONVG = .TRUE.
00101 51* TT = EXP(TLM)
00101 52* GO TO 51
00101 53* 81 TTT(NPT) = TT
00101 54* SSUM(NPT) = SUMS
00101 55* HSUM(NPT) = TT * SUMH
00101 56*
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DATE 101560

FROZEN

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00171 560      GAMMAS(MPT) = CPSUM/(CPSUM-1./UM(MF2))
00172 570      ULM(MPT) = RVROT/(UM(MF2)*PP)
00173 580      UM(MPT) = UM(MF2)
00174 590      OLAPT(MPT) = -1.
00175 600      OLATP(MPT) = 1.
00176 610      TOTN(MPT) = TOTN(MF2)
00177 620      APP(MPT) = PP
00200 630      CPR(MPT) = CPSUM
00201 640      IF (TT.LT.(TLOW-150.1160 TO 903
00203 650      IF (INC.EQ. 0) RETURN
00205 660      INC = 0
00206 670      DO 901 J = 1, NS
00211 680      IF (IUSE(J).EQ. 0 .OR. IUSE(J).EQ. - 10000) GO TO 901
00213 690      INC = INC+1
00214 700      IF (EN(J,MF2).LE. 0.0) GO TO 901
00216 710      IF (TT.LT.TEMP(INC,1)-50. .OR. TT.GT.TEMP(INC,2)+50.) GO TO 903
00220 720      901 CONTINUE
00222 730      RETURN
00223 740      903 TT=0.
00224 750      MPT= MPT+1
00225 760      RETURN
00226 770      END

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FROZEN

END OF COMPILATION: NO DIAGNOSTICS.

SHOG.P GAMEFF

GAMEFF

DATE 101500

PAGE 1

TOP.S GAMEFF, GAMEFF
MSA C3 -10/15/80-13:06:42 (2.)

SUBROUTINE GAMEFF ENTRY POINT 000176

STORAGE USED: CODE(1) 000217; DATA(1) 000044; BLANK COMMON(2) 000000

EXTERNAL REFERENCES (BLOCK, NAME)

0003 XPRR
0004 SORT
0005 MERRIS

STORAGE ASSIGNMENT BLOCK, TYPE, RELATIVE LOCATION, NAME

0001	060014	10L	0001	000025	1.86	0001	000132	20L	0001	000152	5H	000C	R	000002	AMR
0000	R	000006	CFA	0000	R	000005	CGAM	0000	R	000001	G	0000	R	000004	GM
0000	I	000000	I	0000		0000014	INJPS								

00101	10															000025
00103	20															000025
00103	30															000025
00104	40															000025
00107	50															000025
00110	60															000025
00111	70															000025
00113	80															000025
00114	90															000025
00115	100															000025
00116	110															000025
00117	120															000025
00120	130															000025
00122	140															000025
00124	150															000025
00126	160															000025
00127	170															000025
00130	180															000025
00131	190															000025
00132	200															000025
00134	210															000025
00136	220															000025
00137	230															000025
00140	240															000025
00141	250															000025
00143	260															000025
00144	270															000025

END OF COMPILATION: NO DIAGNOSTICS.

DATE 101500 PAGE 2

GAUSS

8406, P

FOR S GAUSS GAUSS
HSA E3 -10/15/88-13:06:54 (7.1)

SUBROUTINE GAUSS ENTRY POINT 000411

STORAGE USED: CODE(11) 000431: DATA(0) 000126: BLANK COMMON(2) 000000

COMMON BLOCKS:

0003 DO, BLE 001560
0004 INDX 000041

EXTERNAL REFERENCES (BLOCK, NAME)

0005 MEMR38

STORAGE ASSIGNMENT (BLOCK, TYPE, RELATIVE LOCATION, NAME)

0001	000107	10L	0001	000011	1106	0001	000043	1206	0001	000062	1276	0001	000130	1526
0001	000161	1676	0001	000204	1176	0001	000115	181	0001	000286	2106	0001	000287	2136
0001	000141	22L	0001	000361	23L	0001	000333	2316	0001	000167	31L	0001	000275	45L
0000	000103	47L	0004	000040	CONV6	0003	000020	8L	0004	000101	9L	0004	000036	CALCH
0000	000000	COEFX	0004	000001	CONV6	0003	000000	6	0004	000003	HP	0000	000056	I
0004	000030	IC	0004	000000	IOEBUG	0000	000071	INJPS	0004	000023	IONS	0004	000021	IP
0004	000037	IOSAVE	0004	000016	IOI	0004	000005	ISV	0004	000034	IT	0004	000015	IUSE
0000	000054	IUSE1	0000	000057	J	0004	000026	JL10	0004	000025	JSL	0004	000031	J51
0000	000061	K	0004	000014	KMAT	0004	000040	LSAVE	0004	000006	MOLES	0004	000024	MC
0004	000022	NEUR	0004	000035	MFZ	0004	000012	NLM	0000	000055	NM	0004	000017	NOF
0004	000020	NOMIT	0004	000007	MP	0004	000011	NPT	0004	000027	NREAC	0004	000013	MS
0004	000010	NT	0004	000033	SHOCK	0004	000004	SP	0000	000050	SUM	0000	000060	TEMP
0004	000002	TP	0004	000032	VOL	0003	000150	X	0000	000052	Z			

B-46

00101	1*	SUBROUTINE GAUSS	000000
00103	2*	COMMON/DOUBLE/6(20,21),X(20)	000000
00104	3*	COMMON/INDX/ IOEBUG, CONV6, TP, P, SP, ISV, MOLES, MP, ANI, NPT, NLM, NS, /INDX/	000000
00104	4*	1 KMAT, IUSE, IOI, NCF, NOMIT, IP, NEUR, IONS, NC, JSL, JL10, /INDX/	000000
00104	5*	2 NREAC, IC, J51, VOL, SHOCK, IT, NFZ, CALCH, IOSAVE, LSAVE /INDX/	000000
00105	6*	DOUBLE PRECISION COEFFX(20), G, SUM, X, Z	000000
00105	7*	C BEGIN ELIMINATION OF MNTH VARIABLE	000000
00106	8*	IUSE1=IUSE+1	000000
00107	9*	DO 45 NM = 1, IUSE	000000
00112	10*	IF (NM .NE. IUSE1) GO TO 8	000002
00114	11*	IF (G(MN, NM)) 31, 23, 31	000011
00114	12*	C SEARCH FOR MAXIMUM COEFFICIENT IN EACH ROW	000014
00117	13*	DO 10 I=NM, IUSE	000020
00122	14*	COEFFX(I) = 1.0E38	000047
00123	15*	IF (G(I, NM).EQ.0.) GO TO 10	000051
00125	16*	COEFFX(I) = 0.	000054
00126	17*	DO 10 J=NM, IUSE1	000062

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OF POOR QUALITY

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00131 180 SUM = G(I,J) 000062
00132 190 IF (SUM.LT.0.) SUM=-SUM 000064
00133 200 IF (J.NE.MN) GO TO 9 000072
00134 210 Z = SUM 000075
00135 220 GO TO 10 000077
00136 230 9 IF (SUM.GT.COEFX(I)) COEFX(I)=SUM 000101
00137 240 10 CONTINUE 000111
00138 250 COEFX(I) = COEFX(I)/Z 000111
00139 260 10 CONTINUE 000121
00140 270 TEMP = 1.0E38 000121
00141 280 I=0 000123
00142 290 DO 22 J = MN,IUSE 000130
00143 300 IF (COEFX(J).GE. TEMP) GO TO 22 000130
00144 310 TEMP = COEFX(J) 000134
00145 320 I=J 000136
00146 330 22 CONTINUE 000143
00147 340 IF (I.EQ. 0) GO TO 23 000143
00148 350 INDEX I LOCATES EQUATION TO BE USED FOR ELIMINATING THE NTH 000143
00149 360 VARIABLE FROM THE REMAINING EQUATIONS 000143
00150 370 C INTERCHANGE EQUATIONS I AND MN 000145
00151 380 IF (MN.EQ. 1) GO TO 31 000150
00152 390 DO 30 J = MN,IUSE1 000150
00153 400 Z=G(I,J) 000161
00154 410 G(I,J)=G(MN,J) 000162
00155 420 30 G(MN,J) = Z 000164
00156 430 C 30 DIVIDE NTH ROW BY NTH DIAGONAL ELEMENT AND ELIMINATE THE NTH 000164
00157 440 C VARIABLE FROM THE REMAINING EQUATIONS 000167
00158 450 31 K = MN + 1 000171
00159 460 DO 36 J = K, IUSE1 000171
00160 470 IF (G(MN,MN).EQ.0.) GO TO 23 000204
00161 480 36 G(MN,J) = G(MN,J)/G(MN,MN) 000207
00162 490 IF (K.EQ. IUSE1) GO TO 45 000214
00163 500 DO 44 I = K, IUSE 000217
00164 510 DO 44 J = K, IUSE1 000257
00165 520 G(I,J) = G(I,J) - G(I,MN)*G(MN,J) 000257
00166 530 45 CONTINUE 000300
00167 540 C BACKSOLVE FOR THE VARIABLES 000300
00168 550 K = IUSE 000300
00169 560 47 J = K + 1 000300
00170 570 X(K) = 0.000 000303
00171 580 SUM = 0.0 000305
00172 590 IF (IUSE.LT. J) GO TO 51 000312
00173 600 DO 50 I = J, IUSE 000313
00174 610 SUM = SUM + G(I,K)*X(I) 000316
00175 620 51 X(K) = G(M,IUSE1) - SUM 000333
00176 630 K = K - 1 000340
00177 640 IF (K.NE. 0) GO TO 47 000350
00178 650 RETURN 000353
00179 660 23 IUSE = IUSE-1 000361
00180 670 END 000363
00181 680 000430

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6AUSS

8HDG,P

HCALC

DATE 101500

PAGE

3

MCALC

FOR S MCALC, MCALC
HSA E3 -10/15/80-13:06:50 (11.1)

SUBROUTINE MCALC ENTRY POINT 000526

STORAGE USED: CODE(11) 000542; DATA(0) 000066; BLANK COMMON(2) 000000

COMMON BLOCKS:

0003 CONSTS 000004
0004 HOLCOM 000010
0005 POINTS 000101
0006 SPECES 017106
0007 MISC 001701
0010 INDY 000041
0011 CCC 000003

EXTERNAL REFERENCES (BLOCK, NAME)

0012 CPHS
0013 ALG
0015 MDOUS
0016 MIO28
0016 MERR38

STORAGE ASSIGNMENT (BLOCK, TYPE, RELATIVE LOCATION, NAME)

0001	000070	1436	0001	000107	15L	0001	000131	16L	0001	000198	18G	0001	000154	1726
0001	000162	1776	0001	000204	2106	0001	000275	2276	0001	000198	38L	0001	000026	4L
0001	000177	50L	0001	000432	500L	0001	000251	55L	0001	000265	56L	0001	000307	70L
0001	000467	75L	0000	000010	76F	0001	000477	80L	0000	000024	85F	0001	000037	9L
0001	000312	90L	0006	R 011052	A	0004	I 002001	AG	0007	R 000490	AM	0007	R 000705	AM1
0000	R 000002	AMM	0007	R 001135	ANUM	0003	000000	ATMM	0007	000004	ATOM	0004	I 000004	BLK
0007	000514	80	0007	000545	80P	0010	L 000036	CALCH	0006	000000	COEF	0010	000001	CONVG
0005	000032	CPR	0007	R 000706	CPR1	0007	R 000634	CPSUM	0007	R 000634	DATA	0006	010624	DELM
0011	000002	DEMAND	0007	001560	DEMS	0005	000064	DLVPT	0005	000047	DLVTP	0006	R 000312	EM
0004	000000	END	0000	R 000007	ENJ	0006	010150	ENLM	0007	001700	EMLSAV	0007	000000	ENM
0007	001676	EMML	0007	001677	EMSAVE	0007	R 001914	ENTH	0007	000018	EQRAT	0007	I 001948	FAZ
0007	I 001527	FOX	0003	000001	GMET	0011	000000	GRAPH	0010	000003	HP	0007	R 000642	MPP
0007	R 000037	HSUBO	0005	000000	MSUM	0006	R 010376	MO	0000	I 000005	I	0010	000030	IC
0010	000000	IOEBUG	0004	000002	IE	0010	000015	IMAT	0000	000044	INJPS	0010	000023	IONS
0010	000021	IP	0010	000037	ISAVE	0010	000016	IOI	0000	I 000004	IS	0010	000008	ISV
0010	000034	IT	0006	I 016266	IUSE	0004	I 000003	IZERO	0010	I 000031	J	0010	000026	JL10
0011	I 000001	JOUT	0010	000025	JSOL	0000	I 000004	K	0010	000014	KMAT	0010	I 000012	L
0007	I 000063	LLMT	0010	000040	LSAVE	0004	000005	MOL	0010	L 000006	MOLES	0000	I 000003	M
0007	I 000707	NAME	0010	000024	MC	0010	000022	MEWR	0010	000035	MF2	0010	000017	NOF
0010	000020	MOMIT	0010	000007	NP	0010	I 000011	NPT	0010	I 000027	NREAC	0010	I 000013	NS
0000	I 000000	MSP1	0010	000010	NT	0007	I 001135	NUM	0007	R 000635	OF	0004	I 000006	OX
0007	001644	OXF	0003	000002	PATM	0007	R 001363	PECMT	0007	R 000633	PP	0003	R 000003	RBAR
0003	000004	RBR	0007	000644	RH	0010	001611	RHOP	0007	R 001612	RMM	0007	R 001476	RTMP
0003	000005	RVR	0006	R 000644	S	0010	L 000033	SHOCK	0006	016660	SLM	0010	000004	SP
0005	R 000005	SSUM	0006	015364	SUR	0007	000001	SUMM	0007	000003	SD	0006	R 016514	TEMP

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0007 R 000632 THIGH 0007 R 001643 T LN 0007 R 000630 TLOW 0007 R 000627 TM 0007 000631 TMID
0010 000002 TP 0000 R 000001 TSAVE 0000 R 000002 TT 0010 L 000032 VOL
0007 000650 VPLS 0007 R 000652 WP 0004 000007 ZERO

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00101 1* SUBROUTINE HCALC 000000
00102 2* CALCULATE ENTHALPY FOR PROPELLANT USING COEFFICIENTS 000000
00103 3* COMMON /CONSTS/ AMN,GHET,PATM,RBAR,RBR,RVR /CONSTS/ 000000
00104 4* COMMON /MOLCON/ ENO,AG,IE,IZERO,BLK,OL,OX,ZERO /MOLCON/ 000000
00105 5* COMMON/POINTS/ACUM133,SSUM(13),CPR(13),OLVPR(13),OLVPI(13) 000000
00106 6* COMMON/SPECES/COEF(12,7,150),S(150),ENT(150,13),ENLM(150),HOL(150) 000000
00107 7* 1. DELN(150).A(15,150).SUB(150,3).IUG(150).TEMP(150,2).SLN(150) 000000
00108 8* INCLUDE SPECPR 000000
00109 9* COMMON /MISC/ ENN,SUMN,TT,SO,TOM(13,101),LLMT(25),BO(125), 000000
00110 10* BOPI(25,2),TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT, 000000
00111 11* HSUBO,AM(2),HPR(2),RH(2),VMIN(1),VPLS(13),MPI(2), 000000
00112 12* DAT(25),AMI,CPR1,NAME(25,6),ANUM(25,6),PECWT(25), 000000
00113 13* ENTH(25),FAZ(25),RTEMP(25),FOX(25),DEMS(25),RHOP, 000000
00114 14* RMV(25),TLM,OXF(26),ENML,ENSAVE,ENLSAV 000000
00115 15* COMMON /INOX/ IDEBUG,CONVG,TP,MP,SP,ISV,MOLES,MP,NT,NPT,L,NS, 000000
00116 16* KWAT,IMAT,IQ1,MOF,NOMIT,IP,NEUR,IONS,NC,JSOL,JLIO, 000000
00117 17* NREAC,IC,J,VOL,SHOCK,II,MFZ,CALCH,IOSAVE,LSAVE 000000
00118 18* 000000
00119 19* COMMON /CCC/ GRAPH,JOUT,DEMAND 000000
00120 20* 000000
00121 21* DIMENSION NUM(25,6) 000000
00122 22* EQUIVALENCE (ANUM,NUM) 000000
00123 23* INTEGER A6,BLK,FAZ,FOX,OX 000000
00124 24* LOGICAL CALCH,MOLES,SHOCK,VOL 000000
00125 25* TSAVE = TT 000000
00126 26* IF (AM(1).GT. 0.0 .AND. AM(2).GT. 0.0) GO TO 4 000001
00127 27* AM1 = AM(2) 000001
00128 28* IF (AM(2).LE. 0.0) AM1 = AM(1) 000015
00129 29* GO TO 9 000017
00130 30* 4 AM1=(OF+1)*AM(1)+AM(2)/(AM(1)+OF+AM(2)) 000024
00131 31* 9 TM = 0. 000026
00132 32* IF (PP.FT,0.1) TM = ALOG(PP+AM1) 000037
00133 33* SSUM(NPT) = 0. 000037
00134 34* HPP(1) = 0. 000031
00135 35* HPP(2) = 0. 000053
00136 36* HSUBO = 0. 000054
00137 37* CPRI = 0. 000055
00138 38* AMN = (1.,OF) 000056
00139 39* C LOOP ON REACTANTS. IF OXIDANT, K = 1, IF FUEL, K = 2. 000057
00140 40* DO 900 M=1,NREAC 000070
00141 41* K=2 000070
00142 42* IF (FOXIN).EQ.OX,K=1 000070
00143 43* IF (NAME(N,6).NE.IZERO) GO TO 90 000072
00144 44* IF (.NOT.CALCH) GO TO 15 000077
00145 45* TT = RTEMPIN 000102
00146 46* C IS TT IN RANGE 000104
00147 47* 15 IF (SHOCK) GO TO 16 000107
00148 48* IF (TT.LT. TLOW - 100.0 .OR. TT.GT. THIGH + 1000.0) GO TO 75 000110
00149 49* 16 J=NUMIN(6) 000131

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DATE 101 580

HCALC

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00162 50* IF (J-ME.O) GO TO 90
00163 51* DO 10 J=1,N
00164 52* DATA(J) = 0.0
00165 53* DO 30 I=1,S
00166 54* IF (AMUM(I) -LE. 0.0) GO TO 50
00167 55* DO 20 J=1,L
00168 56* IF (LLMT(J) .EQ. NAME(M,I)) GO TO 30
00169 57* DATA(J) = DATA(J) + AMUM(M,I)
00170 58* DO 10 J=1,N
00171 59* IF (IUSE(J) .EQ. 0) GO TO 55
00172 60* IS = IS+1
00173 61* IF (FAZ(M) .EQ. AG) GO TO 70
00174 62* IF (IT-6T) .TEMP (IS,2) .AND. TEMP (IS,2) .NE. THIGH) GO TO 70
00175 63* IF (IT-6T) .TEMP (IS,1) .AND. TEMP (IS,1) .NE. TLOW) GO TO 70
00176 64* GO TO 56
00177 65* 55 IF (FAZ(M) .NE. AG .AND. FAZ(M) .NE. BLK) GO TO 70
00178 66* 56 DO 60 I=1,L
00179 67* 60 IF (A(I,J) -ME. DATA(I)) GO TO 70
00180 68* NUM(M,6) = J
00181 69* GO TO 90
00182 70* CONTINUE
00183 71* GO TO 80
00184 72* 90 IF (MOLES) ENJ = PECM(I)/M(P(K))
00185 73* IF (.NOT. MOLES) ENJ = PECM(I)/RNM(M)
00186 74* ENJ = ENJ/ANN
00187 75* IF (K .EQ. 1) ENJ = ENJ*OF
00188 76* IF (NAME(M,6) .NE. IZERO) GO TO 500
00189 77* I = NS
00190 78* NS = J
00191 79* TLN = ALOG(TT)
00192 80* IF (.NOT. CALCM) EN(J,MPT) = ENJ
00193 81* CALL CPHS
00194 82* NS = I
00195 83* IF (MO(J) .GT. -.01 .AND. MO(J) .LT. .01) MO(J) = 0.
00196 84* RTMP(M) = TT
00197 85* IF (VOL) MO(J) = MO(J) -1.
00198 86* ENTH(M) = RBAR*TT*MO(J)
00199 87* CPRI = CPRI + CPSUM
00200 88* 500 HSUBD = HSUBD + ENTH(M)*ENJ
00201 89* HPR(K) = HPR(K) + ENTH(M)*ENJ
00202 90* 900 SSUM(MPT) = SSUM(MPT) + ENJ*(S(I) - ALOG(ENJ) - TM)
00203 91* TT = TSAVE
00204 92* HSUBD = HSUBD/RBAR
00205 93* RETURN
00206 94* 75 WRITE(JOUT,76)
00207 95* 76 FORMAT (//20X,57HREACTANT TEMPERATURE OUT OF RANGE OF THERMO DATA
00208 96* 11M HCALC/)
00209 97* RETURN
00210 98* 80 WRITE(JOUT,85) N
00211 99* 85 FORMAT (//20X,12,42MTH REACTANT IS NOT IN THERMO DATA IN HCALC/)
00212 100* RETURN
00213 101* ENDO
00214 102*

```

END OF COMPILATION: NO DIAGNOSTICS.

MCALC

2406,P

LISTIT

DATE 101500

PAGE

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0PRT.S LISTIT
PURPUR 28R1H E33 570Y11 10/15/80 13:07:03

LISTIT

SEVIGNIN208+TPR(10).LISTIT
 1 2FOR.S LEVIS.BLOCK1, LEVIS.BLOCK1
 2 2FOR.S LEVIS.CPHS, LEVIS.CPHS
 3 2FOR.S LEVI.DETOM, LEVIS.DETOM
 4 2FOR.S LEVIS.FOLBRN, LEVIS.FOLBRN
 5 2FOR.S LEVIS.FROZEN, LEVIS.FROZEN
 6 2FOR.S LEVIS.GAMEFF, LEVIS.GAMEFF
 7 2FOR.S LEVIS.GAUSS, LEVIS.GAUSS
 8 2FOR.S LEVIS.MCALC, LEVIS.MCALC
 9 2FOR.S LEVIS.LTCPS, LEVIS.LTCPS
 10 2FOR.S LEVIS.MAIN, LEVIS.MAIN
 11 2FOR.S LEVIS.MATRIX, LEVIS.MATRIX
 12 2FOR.S LEVIS.OUT1, LEVIS.OUT1
 13 2FOR.S LEVIS.REACT, LEVIS.REACT
 14 2FOR.S LEVIS.RMTOUT, LEVIS.RMTOUT
 15 2FOR.S LEVIS.ROCKET, LEVIS.ROCKET
 16 2FOR.S LEVIS.RREAD, LEVIS.RREAD
 17 2FOR.S LEVIS.SAVE, LEVIS.SAVE
 18 2FOR.S LEVIS.SEARCH, LEVIS.SEARCH
 19 2FOR.S LEVIS.SHCK, LEVIS.SHCK
 20 2FOR.S LEVIS.THERMP, LEVIS.THERMP
 21 2FOR.S LEVIS.VARFMT, LEVIS.VARFMT
 22 2BRKPT PRINTB

2MDG.P LTCPS

ORIGINAL PAGE IS
 OF POOR QUALITY

FOR S LTCPMS.LTCPMS
HSA E3 -10/15/80-13:07:03 (2.1)

SUBROUTINE LTCPMS ENTRY POINT 000205

STORAGE USED: CODE(1) 000221; DATA(0) 000130; BLANK COMMON(2) 000000

COMMON BLOCKS:

0003 CONSTS 000004
0004 LOMTH 001201

EXTERNAL REFERENCES (BLOCK, NAME)

0005 PAGIT
0006 CHRSTZ
0007 GOUT
0010 RDAYAI
0011 ROCHAR
0012 NDCODS
0013 ROATAF
0014 MIOIS
0015 MIOZS
0016 MERRIS

STORAGE ASSIGNMENT (BLOCK, TYPE, RELATIVE LOCATION, NAME)

0001	000006	10L	0000	000072	100F	0001	000025	1246	0001	000045	1326	0001	000111	1446
0001	000113	147G	0001	000124	1566	0001	000026	20L	0001	000051	30L	0001	000122	46L
0003	000000	ATMN	0004	R	000361	CPL	0003	000001	6MET	0004	R	000551	HL	0000
0004	I	001131	ILSP	0000	I	000024	IMN	0000	000107	IMJPS	0000	I	000066	I
0004	I	000015	ITPMN	0000	I	000067	J	0000	I	000071	K	0000	I	000012
0003	000002	PATM	0003	R	000003	RBAR	0003	000004	RBR	0004	I	000000	MLTSP	0000
0004	R	000741	SL	0004	R	000001	SUBLT	0003	000004	R0UM	0004	R	000062	R0UM
				0004	R	000171	TL					0003	000005	RVR

SUBROUTINE LTCPMS		LTCP		10	
00101	1*				000000
00101	2*	C			000000
00101	3*	C			000000
00101	4*	C			000000
00101	5*	C			000000
00103	6*				000000
00103	7*	C			000000
00104	8*				000000
00105	9*				000000
00105	10*				000000
00105	11*	C			000000
00105	12*	C			000000
00106	13*				000000
00106	14*				000000

PROCESS LOW TEMPERATURE CP,H,S (VIA MIPS I/O)

DIMENSION MIPS OUTPUT ARRAYS

DIMENSION INLTMM(10),ISHMN(3),ITPMN(7),IMN(5,6),RDUM(4)

COMMON /CONSTS/ ATMN,GMET,PATM,RBAR,RBR,RVR

COMMON /LOMTH/ MLTSP,SUBLT(40,3),TL(40,3),CPL(40,3),HL(40,3),

I SL(40,3),ILSP(40)

SET DATA FOR MIPS OUTPUT

DATA INLTMM/24HTYPE THE NUMBER OF LOW T,

I 36TEMPERATURE SPECIES TO BE ENTERED /

```

00110 150 DATA ISNMN/18HTYPE SPECIES NAME / 000000
00112 160 DATA ISNMN/2HTYPE NUMBER OF TEMPERATURES, THIS SPECIES 000000
00114 170 DATA ISNMN/3HTYPE TL CPL, ML, SL WHERE 000000
00116 180 1 36M TL-TEMPERATURE 000000
00118 190 2 36M CPL-CONSTANT PRESSURE SPECIFIC HEAT, 000000
00120 200 3 36M ML-ENTHALPY 000000
00122 210 4 36M SL-ENTROPY 000000
00124 220 C NLTSF=0 000000
00126 230 CALL PAGI 000000
00128 240 CALL CHRSTZ17, 000000
00130 250 10 CALL GOUTIMM, 56J, 000002
00132 260 C CALL PDATAT1, NLTSF, 510 000006
00134 270 C LOOP FOR EACH SPECIES 000011
00136 280 C DO 60 I=1, NLTSF 000011
00138 290 CALL GOUTIMM(17) 000016
00140 300 CALL ROCHAB, RDUM, 27-1, 520J 000026
00142 310 DECODE(100, RDUM) (SURL(I, J), J=1, 3) 000031
00144 320 CALL GOUTIMM(42) 000037
00146 330 CALL PDATAT1(1, NT, 530) 000056
00148 340 IF(NT.LT.1 .OR. NT.GT.3) 60 TO 30 000064
00150 350 ILSP(I)=0 000102
00152 360 C LOOP FOR EACH TEMPERATURE 000102
00154 370 DO 50 K=1, NT 000102
00156 380 DO 45 J=1, 5 000103
00158 390 CALL GOUTIMM(J, 1, 36) 000113
00160 400 CONTINUE 000124
00162 410 CONTINUE 000124
00164 420 DO 48 J=1, 4 000124
00166 430 RDUM(J)=0. 000124
00168 440 CONTINUE 000125
00170 450 CALL PDATAT1(4, RDUM, 546) 000125
00172 460 TL(I, K)=RDUM(1) 000132
00174 470 CPL(I, K)=RDUM(2) 000132
00176 480 ML(I, K)=RDUM(3) 000136
00178 490 SL(I, K)=RDUM(4) 000140
00180 500 ILSP(I)=ILSP(I)+1 000142
00182 510 CPL(I, K)=CPL(I, K)/RBAR 000145
00184 520 ML(I, K)=ML(I, K)/IL(I, K)/RBAR 000147
00186 530 SL(I, K)=SL(I, K)/RBAR 000152
00188 540 CONTINUE 000163
00190 550 C END SPECIES LOOP 000163
00192 560 C CONTINUE 000163
00194 570 60 RETURN 000163
00196 580 C 000163
00198 590 100 FORMAT(3A) 000220
00200 600 C END 000220
00202 610 000220
00204 620
00206 630
00208 640
00210 650
00212 660

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LTCPHS

ANDG, P MAIN

DATE 101500

PAGE

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MAIN

DATE 101500

PAGE

1

FROM: MAIN,MAIN
MSA ES -10/15/00-13:07:06 (39.1)

MAIN PROGRAM

STORAGE USED: CODE(1) 001514: DATA(1) 000720: BLANK COM(1) 000000

COMMON BLOCKS:

0003 CONSTS 000004
0004 MOLCOM 000010
0005 PRIMIS 000135
0006 SPECES 017106
0007 MISC 001701
0010 IMOX 000041
0011 PERF 000166
0012 CCC 000003
0013 FUEL 000004
0014 MIN2 000002

EXTERNAL REFERENCES (BLOCK, NAME)

0015 DYES
0016 PSIMT
0017 PAGIT
0020 CHRSTZ
0021 GOUT
0022 ROATAI
0023 AREAD
0024 COALCY
0025 LYCPMS
0026 ROCHAR
0027 MDC008
0030 MOVABS
0031 MOLOTT
0032 REACT
0033 SEARCH
0034 THERMP
0035 DETON
0036 ROCKET
0037 SNCR
0040 NPSTRM
0041 MINTPS
0042 MV0US
0043 MIOZS
0044 MERR2S
0045 MREVS
0046 MR0US
0047 MIO38
0050 MIO18
0051 MRLS
0052 MURLS
0053 MVERFS
0054 AL06
0055 MSTOP5

DATE 10150

MAIN

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00103 40 COMMON /MOLCOM/ END,GAS,IE,IZ,BLANK,MOL,OR,ZERO 000001
00104 50 COMMON/POINITS/MSUM(13),SUM(13),CPRI(13),DLVTP(13),DLVPT(13) 000001
00105 60 1 .GAMMAS(13),PI(26),T(26),V(13),PP(13),MW(13),SOMVEL(13),TTT(13), 000001
00106 70 2 .VLM(13),TOTM(13) 000001
00107 80 COMMON/SPECES/COEF(12,7,15),S(150),ENI(50,13),TMLM(150),MO(150) 000001
00108 90 1 .DELM(150),A(15,150),SUB(150,13),IUSE(150,13),TEMP(150,21),SLM(150) 000001
00109 100 INCLUDE SPECPR 000001
00110 110 COMMON /MISC/ ENH,SUM,TT,S,ATOM(13,101),LLMT(25),BO(25), 000001
00111 120 BOPI(25,2),TM,TLOW,TM2D,TIEM,PP,COSUM,OF,EGRAT, 000001
00112 130 MSUBQ,AM(2),MPP(2),RM(2),VM(2),VPLS(2),MP(2), 000001
00113 140 DATA(25),AM1,CPRI,NAME(25,6),ANUM(13,6),PECVT(25), 000001
00114 150 ENI(25),E(2,25),ATEMP(25),FOX(25),OEN(15),RMOP, 000001
00115 160 RM(25),TLM,OFF(25),ENML,SENSAVE,ENLSAV 000001
00116 170 COMMON /INOX/ IDEBUG,CONVG,IP,MP,SP,ISV,MOLES,MP,MT,NPT,L,MS, 000001
00117 180 WREAC,IC,J31,VOL,SHOCK,II,MF2,CALCM,IOSAVE,LSAVE 000001
00118 190 COMMON /PERF/ PCP(26),VMOC(13),SPIM(13),VACI(13),SUBAR(13), 000001
00119 200 SUPAR(13),APPI(13),AEAT(13),EOL 000001
00120 210 1 000001
00121 220 C 000001
00122 230 COMMON /CCC/ GRAPH,JOUT,DEMAND 000001
00123 240 COMMON /CFUEL/CF,MWV,UCP,PER 000001
00124 250 COMMON /NIN2/M1,M2 000001
00125 260 INTERP BLANK,DATA,END,INSERT,OMIT,REAC,SUB,THRM 000001
00126 270 DIMENSION NIN(150) 000001
00127 280 DATA (NIN(1),I=1,81)/ 000001
00128 290 X*ALC(1,1),,ALU(1,1),, 000001
00129 300 X*ALC(1,2),,ALU(1,2),, 000001
00130 310 X*ALN(1,1),,ALU(1,1),, 000001
00131 320 X*ALN(1,2),,ALU(1,2),, 000001
00132 330 X*CS(1,1),,ALU(1,1),, 000001
00133 340 X*CS(1,2),,ALU(1,2),, 000001
00134 350 X*SI(1,1),,ALU(1,1),, 000001
00135 360 X*SI(1,2),,ALU(1,2),, 000001
00136 370 X*SI(1,3),,ALU(1,3),, 000001
00137 380 X*SI(1,4),,ALU(1,4),, 000001
00138 390 X*SI(1,5),,ALU(1,5),, 000001
00139 400 X*SI(1,6),,ALU(1,6),, 000001
00140 410 X*SI(1,7),,ALU(1,7),, 000001
00141 420 X*SI(1,8),,ALU(1,8),, 000001
00142 430 X*SI(1,9),,ALU(1,9),, 000001
00143 440 X 000001
00144 450 DATA INSERT,MIT,MW,REAC,THRM,NINSE,OMIT,NAME,SHREAC,NUMBER/ 000001
00145 460 DATA MLOW/MLOW, 000001
00146 470 DIMENSION INSERT(13,3),NCD(4),OMIT(13,3) 000001
00147 480 DIMENSION RMUM(2) 000001
00148 490 EQUIVALENCE (DELM,ENI,ENML,OMIT),ENI,OFF(1,OF,OFFL),ISO,SOI 000001
00149 500 LOGICAL CALC4,OFM,COLRATIO,FA,FPCT,MP,IONSP,MOLES,MEAN, 000001
00150 510 MSOM,OF,PSIA,RT,SPOCK,SP,SV,TP,TU,UV,VOL 000001
00151 520 C 000001
00152 530 LOGICAL ROVFS,FIRST 000001
00153 540 C 000001
00154 550 REAL MIX(26) 000001
00155 560 C 000001
00156 570 NAMELIST /IMPT2/ DETM,RATIO,FA,FPCT,MP,IONSP,MIX,MMS,MSOM, /IMPT2/ 000001
00157 580 OF,P,PSIA,RT,SO,SHOCK,SO,SP,SV,T,TP,TU,UV,V 000001
00158 590 DATA INAM/10/ 000001
00159 600 000001

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ORIGINAL PAGE IS
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00142 60* C
00143 61* FIRST=.TRUE.
00144 62* CALL MPSINT
00145 63* CF=.1.0
00146 64* N1=0
00147 65* N2=0
00148 66* 1 WRITE(JOUT,400)
00149 67* DO 100 I=1,6
00150 68* MIX(I)=0.0
00151 69* P(I)=0.
00152 70* T(I)=0.
00153 71* 300 V(I)=0.0
00154 72* TP=.FALSE.
00155 73* HP=.TRUE.
00156 74* TV=.FALSE.
00157 75* UV=.FALSE.
00158 76* SV=.FALSE.
00159 77* RNI=.FALSE.
00160 78* SO=0.0
00161 79* SP=.FALSE.
00162 80* SMOCK=.FALSE.
00163 81* DETN=.FALSE.
00164 82* MMW=.FALSE.
00165 83* PSIA=.TRUE.
00166 84* NSOM=.FALSE.
00167 85* IONS=.FALSE.
00168 86* IDEBUG=0
00169 87* FA=.FALSE.
00170 88* OF=.TRUE.
00171 89* ERATIO=.FALSE.
00172 90* FPCT=.FALSE.
00173 91* EOL=.TRUE.
00174 92* NEUR=.FALSE.
00175 93* 400 FORMAT(1H1)
00176 94* 2 CONTINUE
00177 95* NREAC=0
00178 96* NSERT=0
00179 97* NOMIT=0
00180 98* CALL PAGIT
00181 99* JOUT=6
00182 100* IF IRDYES(*TYPE YES FOR PRINT TO PRINT FILE*,35)) JOUT=31
00183 101* 203 CONTINUE
00184 102* CALL PAGIT
00185 103* CALL CHRSLZ(1)
00186 104* CALL GOUT('LEWIS CHEMICAL EQUILIBRIUM PROGRAM',34)
00187 105* CALL GOUT(' ',1)
00188 106* CALL GOUT(' MAIN MENU',19)
00189 107* CALL GOUT(' ',1)
00190 108* CALL GOUT(' 1 - INSERT THERMODYNAMICS DATA',31)
00191 109* CALL GOUT(' 2 - INSERT LOW TEMP EXTENSION THERMO DATA',42)
00192 110* CALL GOUT(' 3 - INSERT OR EDIT REACTANTS',29)
00193 111* CALL GOUT(' 4 - OMIT SPECIES FROM THERMO DATA',34)
00194 112* CALL GOUT(' 5 - INSERT CONDENSED SPECIES',29)
00195 113* CALL GOUT(' 6 - INSERT OR EDIT NAMELIST',28)
00196 114* CALL GOUT(' 7 - START PROGRAM CALCULATION',30)
00197 115* CALL GOUT(' 8 - INSERT OR EDIT COAL DATA',29)
00198 116*
00199 117*
00200 118*
00201 119*
00202 120*
00203 121*
00204 122*
00205 123*
00206 124*
00207 125*
00208 126*
00209 127*
00210 128*
00211 129*
00212 130*
00213 131*
00214 132*
00215 133*
00216 134*
00217 135*
00218 136*
00219 137*
00220 138*
00221 139*
00222 140*
00223 141*
00224 142*
00225 143*
00226 144*
00227 145*
00228 146*
00229 147*
00230 148*
00231 149*
00232 150*
00233 151*
00234 152*
00235 153*
00236 154*
00237 155*
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00240 1160 CALL GOUT(' RETURN - TERMINATE PROGRAM',27)
00241 1170 ICARD=0
00242 1180 CALL CHRSTZ(4)
00243 1190 CALL READ(1,ICARD,S2D3)
00244 1200 IF (ICARD-EQ-0) GO TO 3
00245 1210 IF (ICARD-NE-0) GO TO 201
00246 1220 GO TO 190,39,11,205,108,210,215,15),ICARD
00247 1230 C
00248 1240 C
00249 1250 CALL SUBROUTINE TO READ REACTANT CARDS
00250 1260 11 CALL READIFIRST)
00251 1270 GO TO 203
00252 1280 C
00253 1290 C
00254 1300 15 CALL COALCVIFIRST)
00255 1310 GO TO 203
00256 1320 C
00257 1330 C
00258 1340 READ LOW TEMPERATURE EXTENSION THERMO DATA
00259 1350 39 CALL LTCFMS
00260 1360 GO TO 201
00261 1370 C
00262 1380 C
00263 1390 READ THERMO DATA FROM CARDS AND STORE ON TAPE
00264 1400 90 NEW = .TRUE.
00265 1410 REMIND
00266 1420 CALL GOUT('ADD THERMO DATA HERE',20)
00267 1430 READ(1,10,IMQ,IMH)
00268 1440 5 FORMAT (3F10.3)
00269 1450 WRITE (4,5) TLOW,TMID,THIGH
00270 1460 97 READ (5,10) (DATA(I),I=1,16),MCD(1)
00271 1470 10 FORMAT(3A9,2A3,4(A2,F3.0),A1,2F10.3,I5)
00272 1480 IF (DATA(1)-EQ-BLANK) DATA(1)=END
00273 1490 WRITE (4,10) (DATA(I),I=1,16)
00274 1500 IF (DATA(1)-EQ-END) GO TO 203
00275 1510 READ (5,20) (DATA(I),I=1,5),MCD(2),(DATA(J),J=6,10),MCD(3),
00276 1520 1
00277 1530 (DATA(I),I=1,14),MCD(4)
00278 1540 20 FORMAT(5E15.8,15/5E15.8,15/4E15.8,120)
00279 1550 WRITE (4,21) (DATA(I),I=1,14)
00280 1560 21 FORMAT(5E15.8/5E15.8/4E15.8)
00281 1570 DO 25 I=1,4
00282 1580 IF (MCD(I)-EQ-1) GO TO 25
00283 1590 WRITE(JOUT,22) (DATA(J),J=1,3)
00284 1600 22 FORMAT(20HERROR IN ORDER OF CARDS FOR ,3A9)
00285 1610 25 CONTINUE
00286 1620 GO TO 97
00287 1630 C
00288 1640 C
00289 1650 CHECK INSERT CARDS
00290 1660 108 CONTINUE
00291 1670 CALL PAGIT
00292 1680 CALL GOUT('TYPE SPECIES TO INSERT(1 PER LINE)',34)
00293 1690 181 CONTINUE
00294 1700 CALL ROCMAR(ROUM,2,-1,9203)
00295 1710 INSERT=INSERT+1
00296 1720 DECODE (207,ROUM) (INSERT(I,INSERT),I=1,3)
00297 1730 GO TO 181
00298 1740 C
00299 1750 C
00300 1760 CHECK OMIT CARDS
00301 1770 CONTINUE
00302 1780 CALL PAGIT
00303 1790
00304 1800
00305 1810
00306 1820
00307 1830
00308 1840
00309 1850
00310 1860
00311 1870
00312 1880
00313 1890
00314 1900
00315 1910
00316 1920
00317 1930
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00320 1960
00321 1970
00322 1980
00323 1990
00324 2000
00325 2010
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00361 172* CALL GOUT('TYPE SPECIES TO OMIT FROM THERMO DATA',37) 000445
00362 173* CONTINUE 000452
00363 174* CALL RDOCHAR,ROUM,2,-1,$200) 000452
00364 175* NOMIT=NOMIT+1 000457
00365 176* DECODE (207,ROUM) (OMIT(I,NOMIT),I=1,3) 000462
00373 177* FORMAILIAN) 000493
00374 178* GO TO 206 000503
00375 179* 200 CONTINUE MAIN00062
00376 180* NEWR=.TRUE. 000505
00377 181* REWIND 4 000506
00400 182* GO TO 203 000511
00400 183* C 000511
00400 184* C BEGIN NAMELIST INPT2 000511
00401 185* 210 CALL PAGIT 000513
00402 186* IF (.NOT.ROYES('TYPE YES FOR PRINT INPT2 NAMELIST',35)) GO TO 1211 000514
00402 187* C ACCESS THE ORIGINAL NAMELIST FROM PREVIOUS RUN 000514
00403 188* REWIND INAM 000521
00405 189* READ INAM,INPT2 000521
00410 190* WRITE (6,INPT2) 000530
00413 191* GO TO 1212 000534
00413 192* C RESET ALL PARTS OF NAMELIST 000534
00414 193* 1211 DO 1210 I=1,26 000540
00417 194* MIX(I)=0 000540
00420 195* PI=0 000540
00421 196* T(I)=0 000541
00422 197* 1220 TP=.FALSE. 000542
00424 198* HP=.TRUE. 000544
00425 199* TV=.FALSE. 000545
00426 200* UV=.FALSE. 000547
00427 201* SV=.FALSE. 000550
00430 202* RKT=.FALSE. 000551
00431 203* SO=0.0 000552
00432 204* SP=.FALSE. 000553
00433 205* SHOCK=.FALSE. 000554
00434 206* DETN=.FALSE. 000555
00435 207* MMHG=.FALSE. 000556
00436 208* PSIA=.TRUE. 000557
00437 209* NSOM=.FALSE. 000560
00440 210* IONS=.FALSE. 000562
00441 211* IDEBUG=0 000563
00442 212* FA=.FALSE. 000564
00443 213* OF=.TRUE. 000565
00444 214* ERATIO=.FALSE. 000566
00445 215* FPCT=.FALSE. 000570
00446 216* GO TO 11211 000571
00447 217* 1212 IF (.NOT.ROYES('TYPE YES TO CHANGE NAMELIST',27)) 000572
00450 218* X GO TO 203 000574
00450 219* 11211 WRITE (6,211) 000574
00452 220* 211 FORMAT(' BEGIN NAMELIST INPT2 INPUT') 000601
00454 221* 2211 CONTINUE 000605
00455 222* READ(5,INPT2) 000605
00456 223* STORE NAMELIST 000605
00456 224* C REWIND INAM 000611
00461 225* WRITE INAM,INPT2 000614
00462 226* ENDFILE INAM 000620
00465 227*

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MAIN00066

00066	220	CALL MOVABS(800,50)	000623
00067	229	CALL MOLDIT	000627
00068	230	GO TO 203	000631
00071	231	215 CONTINUE	000633
00072	232	FIRST=.FALSE.	000633
00073	233	CALL PAGIT	000633
00074	234	CALL GOUT(' ',1)	000635
00075	235	REIND INAM	000641
00076	236	READ (INAM,INPT2)	000644
00077	237	WRITE (6,INPT2)	000650
00078	238	CALL MOVABS(500,50)	000654
00079	239	CALL MOLDIT	000660
00080	240	CALL PAGIT	000662
00081	241	CALL GOUT(' ',1)	000664
00082	242	CALL REACT	000670
00083	243	IF (CF) 1215	000672
00084	244	IF (NOT,MOVES('TYPE YES FOR SPECIAL OMITS FOR COAL DATA',40))	000675
00085	245	X GO TO 1215	000675
00086	246	DO 12 I=1,27	000706
00087	247	DO 12 J=1,3	000714
00088	248	12 OMIT(J,NOMIT,I)=NOMTS(I,3-3-J)	000721
00089	249	NOMIT=NOMIT+27	000727
00090	250	1215 CALCH=.FALSE.	000733
00091	251	DO 755 I=1,MREAC	000733
00092	252	IF (NAME(I,6),EQ,12) CALCH=.TRUE.	000740
00093	253	755 CONTINUE	000746
00094	254	IF (ERATIO) GO TO 213	000746
00095	255	IF (CF) 213	000750
00096	256	DO 212 I=1,26	000756
00097	257	212 MIX(I)=MIX(I)*CF	000754
00098	258	213 IF (PER-1.0),214,	000762
00099	259	MSERT=MSERT+1	000764
00100	260	ENSTRT(1,MSERT)=ICIS	000770
00101	261	ENSTRT(2,MSERT)=	000772
00102	262	ENSTRT(3,MSERT)=	000774
00103	263	214 CONTINUE	000772
00104	264	RMOP=0.	000777
00105	265	VOL=.FALSE.	000777
00106	266	MT=1	001000
00107	267	IF (NOT,TV,AND,.NOT,UV,AND,.NOT,SV) GO TO 304	001002
00108	268	VOL=.TRUE.	001007
00109	269	DO 1304 I=1,26	001014
00110	270	IF (P(I),GT,0.0) P(I)=1.0/P(I)	001014
00111	271	IF (V(I),GT,0.0) P(I)=V(I)	001022
00112	272	IF (P(I),LE,0.0) GO TO 1305	001027
00113	273	1304 MP = I	001032
00114	274	1305 TP = TV	001037
00115	275	MP = UV	001040
00116	276	SP = SV	001042
00117	277	GO TO 322	001044
00118	278	304 DO 305 I=1,26	001050
00119	279	IF (P(I),LE,0.0) GO TO 322	001050
00120	280	MP = I	001053
00121	281	IF (MHP) P(NP) = P(MP)/760.	001057
00122	282	IF (PSIA) P(NP) = P(MP)/PATH	001065
00123	283	305 IF (NSOM) P(NP) = P(MP)/ATM	001073

MAIN0090

MAIN

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00624 28* 322 DO 307 IT = 1,26 001106
00627 285* IF (IT) .LE. 0.0) GO TO 722 001106
00631 286* IF (CF+1.0) .307, 001111
00634 287* Y(I) = Y(I) - 32.0) / 1.8 * 273.15 001114
00635 288* MT = IT 001122
00637 289* DO 425 IST = 1,26 001130
00642 290* IF (MIX(IST) .GT. 0.0) GO TO 323 001130
00644 291* IF (IST.M.1) GO TO 745 001133
00646 292* WRITE(JOUT,724) 001136
00650 293* FORMAT (//,5X,OHNO INPT2 VALUE GIVEN FOR FA, FPCT, OR OF//) 001143
00651 294* IF (MPI2) .GT. 0.0) OXFL = MP(1)/MP(2) 001143
00653 295* GO TO 333 001151
00654 296* 323 OXFL=MIX(IST) 001153
00655 297* IF (FA) OXFL = 1.0 / MIX(IST) 001154
00657 298* IF (FPC) OXFL = 100.0 - MIX(IST) / 001161
00661 299* IF (NOT-ERATIO) GO TO 333 001167
00663 300* ERAT = MIX(IST) 001171
00664 301* IF (ERAT.EQ.1.0) ERAT = 1.000005 001173
00666 302* OXFL = (-ERAT+VMIN(2)-VPLS(2)) / (VPLS(1)-ERAT+VMIN(1)) 001200
00667 303* 333 OXFL(IST) = OXFL 001211
00670 304* 625 NOF = 15T 001212
00672 305* 745 IF (NOT-IONS .OR. LLMT(L) .EQ. IE) GO TO 746 001217
00674 306* L = L+1 001227
00675 307* IF (LLMT(L).NE.IE) NGWR=.TRUE. 001232
00677 308* REWIND 4 001242
00700 309* LLMT(L) = IE 001245
00701 310* BOP(L,1) = 0. 001250
00702 311* BOP(L,2) = 0. 001251
00703 312* GO TO 748 001252
00706 313* 746 IF (LLMT(L).NE.IE) GO TO 748 001254
00708 314* DO 747 J=1,NS 001257
00711 315* 747 IF (AIL(J) .NE. 0.0) IUSE(J) = - 10000 001267
00714 316* L = L-1 001275
00718 317* 748 IF (NEW) CALL SEARCH 001301
00715 318* C INITIAL ESTIMATES 001301
00717 319* SO = SO/984R 001304
00720 320* ENN = .1 001307
00721 321* ENNL = -2.3025851 001311
00722 322* SUMN = ENN 001313
00723 323* DO 432 J=1,NS 001331
00726 324* IF (IUSE(J).GT.0) IUSE(J) = -IUSE(J) 001331
00730 325* IF (IUSE(J).EQ.-10000.AND.IONS) IUSE(J) = 0 001335
00732 326* EM(J,1) = 0. 001346
00733 327* EMN(J) = 0. 001347
00734 328* IF (IUSE(J).NE.0) GO TO 432 001350
00736 329* EM(J,1) = ENN/IONS - MC) 001352
00737 330* EMN(J) = ALOG10(J,1) 001354
00740 331* 432 CONTINUE 001364
00742 332* IOI = L+1 001364
00743 333* IF (MC.EQ.0.OR.INSERT.EQ.0) GO TO 790 001367
00745 334* DO 302 I=1,NS 001377
00750 335* DO 301 J=1,NS 001416
00753 336* IF (IUSE(J).EQ.0) GO TO 301 001421
00755 337* DO 299 IST = 1,3 001430
00760 338* 299 IF (SUB(J,IST) .NE. ENN(IST,1)) GO TO 301 001430
00763 339* IOI = IOI+1 001437

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MAIN0141
MAIN0145

DATE 101580

MAIN

00764	340*	IUSE(J) = -IUSE(J)	001442
00765	341*	GO TO 302	001444
00766	342*	301 CONTINUE	001452
00770	343*	302 CONTINUE	001482
00772	344*	790 IF (.NOT. TP .AND. .NOT. HP .AND. .NOT. SP) GO TO 791	001452
00773	345*	CALL THERMP	001466
00775	346*	GO TO 800	001460
00776	347*	791 IF (DET) CALL DETON	001462
01000	348*	IF (FRT) CALL ROCKET	001465
01002	349*	IF (SHOCK) CALL SHCK	001471
01004	350*	800 NSRT = 0	001476
01005	351*	CALL MOVARS(600,50)	001476
01006	352*	CALL HOLDIY	001502
01007	353*	GO TO 2	001504
01010	354*	3 CONTINUE	001506
01011	355*	CALL MPSTRM	001604
01012	356*	STOP	001507
01013	357*	END	001513

MAIN0153

END OF COMPILATION: NO DIAGNOSTICS.

AM06.P MATRIX

OF S MATRIX.MATRIX
HSA 23 -10/15/80-13:07:13 (11.)

SUBROUTINE MATRIX ENTRY POINT 001063

STORAGE USED: CODE(1) 001107; DATA(0) 000116; BLANK COMMON(2) 000000

COMMON BLOCKS:

0003 POINTS 000335
0004 SPECIES 017106
0005 MISC 001701
0006 DOUBLE 001560
0007 IMOX 000041

EXTERNAL REFERENCES (BLOCK, NAME)

0010 MERR35

STORAGE ASSIGNMENT (BLOCK, TYPE, RELATIVE LOCATION, NAME)

0001	000102	1246	0001	000103	1276	0001	000126	1406	0001	000215	1446	0001	000244	1610
0001	000672	175L	0001	000677	185L	0001	000453	2176	0001	001611	230L	0001	000567	2446
0001	000606	2476	0001	000623	2576	0001	001026	260L	0001	000757	3036	0001	001023	3176
0001	000276	35L	0001	000344	59L	0001	000372	62L	0001	000376	64L	0001	000511	65L
0001	000405	70L	0004	R 011052	A	0005	000490	AM	0005	000708	AM	0005	001138	ANUM
0005	000004	ATOM	0005	R 000514	BD	0005	000545	BOP	0007	000036	CALCH	0004	000000	COEF
0007	L 000001	CONVG	0003	000032	CPR	0005	000706	CPR1	0005	R 000634	CPSUM	0005	000654	DATA
0004	010624	DELM	0005	001560	DENS	0003	000064	OLVPT	0003	000047	OLVTP	0004	R 004312	EM
0000	P 000013	ENERGY	0004	R 010150	ENLM	0005	001700	ENLSAV	0005	R 000000	ENM	0005	001676	ENML
0005	001677	ENSARE	0005	001414	ENTH	0005	000636	ENRAT	0000	R 000010	F	0005	001443	FAZ
0005	001527	FOX	0006	D 000000	G	0003	000101	GAMMAS	0007	L 000003	HP	0005	000642	HPP
0005	R 000617	HSUBO	0003	R 000000	HSUM	0004	R 010376	MO	0000	I 000003	I	0007	000030	IC
0007	000000	IDEBUG	0007	I 000015	IMAT	0000	000023	INOPS	0007	000023	IONS	0007	000021	IP
0007	000017	IOSAVE	0007	I 000016	IQ1	0000	I 000001	IQ2	0000	I 000002	IQ3	0007	000005	ISV
0007	000034	IT	0004	I 016266	IUSE	0000	I 000007	J	0007	000024	JL10	0007	000028	J50L
0007	000031	J51	0000	I 000004	K	0000	I 000006	KK	0007	I 000014	KMAT	0007	I 000012	L
0005	000463	LLMT	0007	000040	LSAVE	0007	000006	MOLES	0005	000707	NAME	0007	000024	MC
0007	000022	MEWR	0007	000015	MF2	0007	000017	NOF	0007	000020	MMIT	0007	000007	MP
0007	I 000011	MPT	0007	000027	MREAC	0007	I 000013	MS	0000	I 000000	MSPP1	0007	000010	MT
0005	000635	OF	0003	001644	OXF	0003	000116	P	0005	001363	PECWT	0005	000633	PP
0003	000217	PPP	0005	000644	RH	0005	001611	RHOP	0005	001612	RHW	0005	001476	RTEMP
0004	R 004064	S	0007	000033	SHOCK	0004	016660	SLN	0003	000251	SOMVEL	0007	L 000004	SP
0000	R 000012	SS	0000	R 000005	SSS	0003	000015	SSUM	0004	015364	SUB	0005	R 000001	SUMM
0005	R 000003	SO	0003	000150	T	0004	016514	TEMP	0000	R 000012	TERM1	0005	000632	THIGH
0005	001643	TLN	0005	000630	TLOW	0003	R 000627	TM	0005	000631	TMD	0005	000320	TOTN
0007	L 000002	TP	0005	R 000002	TT	0003	000266	TTT	0003	000202	V	0003	000303	VLM
0005	000646	VMIN	0007	L 000032	VOL	0005	000650	VPLS	0003	000234	WM	0005	000652	WP
0006	D 001510	X												

MATRIX

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00202 56*      G(IQ2,IQ1) = G(IQ2,IQ1) + SS
00203 57*      G(IQ2,IQ2) = G(IQ2,IQ2) + H0(J) * SS
00204 58*      G(IQ2,IQ3) = G(IQ2,IQ3) + S(J) - ENLM(J) - TM * F
00205 59*      GO TO 62
00206 60*      59      G(IQ2,IQ2) = G(IQ2,IQ2) + H0(J) * 2 * EN(J,NPT)
00207 61*      IF (CONV6) GO TO 64
00211 62*      G(IQ2,IQ3) = G(IQ2,IQ3) + H0(J) * F
00212 63*      62      G(IQ1,IQ3) = G(IQ1,IQ3) + F
00213 64*      64      G(IQ1,IQ2) = G(IQ1,IQ2) + TERM1
00214 65*      GO TO 65
00215 66*      C      CONDENSED SPECIES
00216 67*      70      KK = KK + 1
00217 68*      DO 75 I = 1,L
00221 69*      6(I,KK) = A(I,J)
00222 70*      75      G(I,KMAT) = G(I,KMAT) - A(I,J) * EN(J,NPT)
00224 71*      6(KK,IQ2) = H0(J)
00225 72*      6(KK,KMAT) = H0(J) - S(J)
00226 73*      HSUM(MPT) = HSUM(MPT) + H0(J) * EN(J,NPT)
00227 74*      IF (NOT SP) GO TO 65
00231 75*      SSS = SSS + S(J) * EN(J,NPT)
00232 76*      6(IQ2,KK) = S(J)
00233 77*      68      CONTINUE
00235 78*      SSS = SSS + G(IQ2,IQ1)
00236 79*      HSUM(MPT) = HSUM(MPT) + G(IQ1,IQ2)
00237 80*      G(IQ1,IQ1) = SUMN - ENN
00238 81*      C      REFLECT SYMMETRIC PORTIONS OF THE MATRIX
00240 82*      K = IQ1
00241 83*      IF (HP .OR. CONV6) K = IQ2
00242 84*      DO 102 I = 1,K
00243 85*      DO 102 J = 1,K
00246 86*      102      G(I,J) = G(I,J)
00251 87*      C      COMPLETE THE RIGHT HAND SIDE
00254 88*      IF (CONVG) GO TO 175
00256 89*      DO 145 I = 1,L
00261 90*      X(I) = 0
00262 91*      145      G(I,KMAT) = G(I,KMAT) + X(I)
00264 92*      6(IQ1,KMAT) = G(IQ1,KMAT) * ENN - SUMN
00265 93*      C      COMPLETE ENERGY ROW AND TEMPERATURE COLUMN
00267 94*      IF (KMAT .EQ. IQ2) GO TO 185
00267 95*      IF (SPIENERGY = 50 + ENN - SUMN - SSS)
00271 96*      IF (HPIENERGY = MSUBO/TT - HSUM(MPT))
00273 97*      175      G(IQ2,IQ3) = G(IQ2,IQ3) + ENERGY
00274 98*      175      G(IQ2,IQ2) = G(IQ2,IQ2) + CPSUM
00275 99*      185      IF (NOT VOL .OR. CONV6) RETURN
00275 100*      C      CONSTANT VOLUME MAX
00277 101*      K = IQ1 - 1
00277 102*      IF (KMAT .EQ. IQ2) GO TO 230
00280 103*      DO 220 I = 1,M
00285 104*      6(IQ1,I) = G(IQ2,I) - G(IQ1,I)
00286 105*      6(I,IQ1) = G(I,IQ2) - G(I,IQ1)
00287 106*      220      G(I,IQ2) = G(I,IQ3)
00287 107*      6(IQ1,IQ1) = G(IQ2,IQ2) - G(IQ1,IQ2) - G(IQ2,IQ1)
00287 108*      6(IQ1,IQ2) = G(IQ2,IQ3) - G(IQ1,IQ3)
00287 109*      IF (HP) 6(IQ1,IQ2) = G(IQ1,IQ2) + ENN
00287 110*      GO TO 260
00287 111*      230      DO 240 I = 1,K
00287 112*

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MATRIX

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00321 1120 240 6(1,101) = 6(1,102)
00322 1130 260 KMAT = IMAT
00323 1140 IMAT = IMAT-1
00324 1150 RETURN
00325 1160 EN
00326 1170
    
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MATN0090

END OF COMPILATION: NO DIAGNOSTICS.

AM06.P OUT1

OUT1

DATE 101500

PAGE 1

3FOR,S OUT1 OUT1
MSA ES -10/15/80-13:07:10 (15,)

SURROUT1E OUT1 ENTRY POINT 002156
OUT2 ENTRY POINT 002141
OUT3 ENTRY POINT 002164
OUT4 ENTRY POINT 002187

STORAGE USED: CODE(1), 002172; DATA(0) 000655; BLANK COMMON(2) 000000

COMMON BLOCKS:

0003 CONSTS 000006
0004 HOLCOM 000010
0005 POINTS 000335
0006 SPECES 017104
0007 MISC 001701
0010 INDX 000041
0011 PERF 000164
0012 CUPT 000073
0013 CC 000003
0014 CFUEL 000004

EXTERNAL REFERENCES (BLOCK, NAME)

0015 VARFMT
0016 MOVABS
0017 HOLDIT
0020 PAGIT
0021 MVDUS
0022 NI018
0023 NI028
0024 NI038
0025 SORT
0026 MERR35

STORAGE ASSIGNMENT (BLOCK, TYPE, RELATIVE LOCATION, NAME)

0000	000371	1F	0001	000034	10L	0001	001440	10146	0001	001443	10206	0001	001470	10346
0001	001477	10426	0001	001510	10456	0001	001520	10506	0001	001564	10646	0001	001573	10726
0001	001621	11076	0001	001627	11156	0001	001643	11246	0001	001673	11356	0001	001752	11536
0001	001760	11416	0001	002010	11766	0001	002042	12056	0001	002054	12146	0001	002066	12236
0001	002100	12326	0001	002112	12416	0001	001044	130L	0001	000025	1546	0001	001120	160L
0001	000043	1646	0001	001144	170L	0001	001152	175L	0001	001221	177L	0001	001257	179L
0001	001261	180L	0000	000377	2F	0000	000333	20F	0001	000112	2006	0001	001334	200L
0001	001371	210L	0001	001373	211L	0000	000353	22F	0000	000310	240F	0001	000213	2476
0001	000235	2616	0001	000276	2776	0000	000406	280F	0000	000422	290F	0001	000036	30L
0000	000450	300F	0000	000452	310F	0001	000320	3106	0000	000416	320F	0001	000314	3216
0001	000362	3326	0000	000412	340F	0001	000404	3436	0001	000420	3506	0001	000447	3646
0001	000471	3756	0001	000501	4036	0001	000522	4146	0001	000544	4256	0001	000560	4326
0001	000606	4456	0001	000645	45L	0001	000623	4556	0001	000647	4716	0000	000471	490F
0000	000472	492F	0001	000217	50L	0001	001481	500L	0001	000670	5026	0000	000477	504F

OUT1

0001	001533	500L	0001	001536	510L	0001	000711	5136	0001	00104	514L	0001	000225	52L
0000	000504	520E	0000	000717	5206	0000	000511	524F	0000	000734	5276	0000	000517	532F
0001	000543	5376	0000	000525	524F	0000	000532	544F	0001	000763	5456	0000	000540	546F
0000	000546	548F	0000	000554	550F	0000	000562	552F	0001	001007	5556	0001	001075	510E
0001	001100	6136	0001	001106	6206	0001	001131	6316	0001	001119	6366	0001	001163	64L
0001	001137	6506	0001	001216	6616	0001	001247	6736	0001	001273	7156	0001	001307	7206
0001	001331	7276	0001	000342	74L	0001	001362	7416	0000	000405	80F	0006	011052	A
0011	000150	AFAT	0007	000640	AM	0007	000705	AM1	0007	001138	ANUM	0011	000133	APP
0003	000000	ATMM	0007	000004	ATOM	0007	000514	80	0007	000545	80P	0010	000036	CALCH
0014	000000	CF	0000	R 000103	CMW	0006	000000	COEF	0000	000047	COF	0010	000001	CONVE
0005	R 000012	CPR	0007	000706	CPA1	0007	000634	CPSUM	0007	000654	CDA	0006	010424	DELV
0013	000002	DEMAND	0007	R 001540	DEMS	0005	R 000644	DLRPT	0005	R 000047	DLVTR	0000	R 000236	DOL
0000	R 000167	EE	0006	R 004312	EM	0004	000000	END	0004	010150	ENLM	0007	001700	ENLSAV
0007	000000	ENM	0007	001676	ENML	0007	001677	ENSAVE	0007	R 001414	ENTM	0011	L 000148	EOL
0007	R 000036	EQRAT	0012	000002	FA	0012	R 000003	FAP	0007	R 001445	FAZ	0012	R 000085	FB
0012	000004	FC	0012	R 000007	FCE	0012	000012	FCEST	0012	000014	FCV	0012	R 000015	FG
0012	00017	FCE	0012	000020	FCE	0012	R 000021	FM	0000	R 000036	FMM	0012	000023	FI
0012	000028	FJY	0012	R 000027	FM	0012	R 000031	FMI	0012	000040	FMM	0012	R 000052	FOUR
0007	I 001527	FOX	0012	000053	FP	0000	R 000046	FPC	0000	R 000047	FPP	0012	R 000049	FS
0000	R 000040	FSS	0012	R 000056	F5V	0012	R 000057	FT	0012	R 000061	FTR	0000	R 000034	FTR
0012	R 000063	FV	0012	R 000065	FVEL	0000	R 000001	FVLM	0012	R 000001	F13	0012	000000	F9X
0005	R 000103	GAMMAS	0004	000001	GAS	0003	000001	GNET	0013	000000	GRAPH	0000	R 000003	HEAD
0000	R 000221	MYSD	0000	R 000152	MVVS	0014	R 000001	MVV	0010	000003	HP	0007	000042	MPP
0007	000037	MSUD	0005	R 000000	MSUM	0006	010374	MD	0000	I 000002	I	0010	000030	IC
0018	000000	IDRUG	0000	I 000261	TD6	0004	000002	IE	0000	I 000050	IFLAG	0000	I 000104	IJ
0010	000015	IMAT	0000	I 000253	INDX	0000	000624	INJPS	0010	000023	IOMS	0018	000021	IP
0004	I 016244	IUSE	0010	000016	I01	0006	I 015364	ISUB	0010	000055	ISV	0010	000034	IT
0010	R 000025	JSOL	0004	000003	I2	0000	I 000045	J	0010	000026	JLIG	0013	I 000001	JOUT
0000	R 000056	LMVD	0010	000031	JS1	0000	I 000043	K	0010	000014	KMAT	0004	I 000004	LAHM
0000	I 000306	L3	0000	R 000051	LMVS	0007	000043	LLMT	0010	000040	LSAVE	0000	I 000005	L1
0007	I 000707	NAME	0000	I 000307	L4	0004	000005	MOL	0010	L 000003	MOLES	0000	I 000014	MV
0010	000012	MLM	0010	000024	MC	0000	I 000044	MO	0010	000022	MEUR	0010	000035	MF2
0010	I 000027	MREAC	0010	000017	MOF	0010	000020	MOHIT	0010	000007	MP	0010	I 000011	MPT
0012	R 000067	OME	0004	I 000013	MS	0000	I 000000	MSPP1	0010	000010	MT	0007	R 000035	OF
0011	000000	PCP	0004	I 000006	OX	0007	001644	OXF	0005	000134	P	0003	R 000002	PATM
0003	R 000003	RBAR	0007	R 001363	PECMT	0014	R 000003	PER	0007	000433	PP	0005	R 000027	PPP
0007	R 001476	RTMP	0003	R 000004	RBR	0007	000644	RM	0007	R 001611	RMOP	0007	001612	RMV
0005	R 000251	SOMVEL	0003	000005	RVR	0004	000644	S	0010	000033	SMOCK	0004	014460	SLM
0011	000101	SUBAR	0000	R 000303	SUM	0007	000001	SUPN	0011	000018	SSUM	0006	R 013364	SUB
0005	000150	T	0006	016514	TEMP	0007	000063	THIGH	0012	000016	SUPAR	0007	000003	SO
0007	000040	TLOW	0007	000427	TH	0007	000631	THID	0005	R 000320	THREE	0007	001643	TLM
0007	000002	TY	0005	R 000266	TYT	0012	R 000071	TW0	0005	R 000202	V	0011	000044	VAC1
0005	R 000303	VLM	0007	000496	VHIM	0011	000032	VMOG	0010	L 000032	VOL	0007	000450	VPLS
0014	R 000002	VCR	0005	R 000234	WM	0007	000652	WP	0000	R 000120	XDP	0000	R 000204	YDP
0000	R 000135	TOPS	0000	R 000020	YM	0000	R 000025	YX	0004	R 010376	Z	0004	000007	ZERO
0012	000072	ZEROF												

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OUTP0001
/CONSIS/
/MOLCON/

SUBROUTINE OUT1
COMMON /CONSIS/ ATMM,GNET,PATM,RBAR,RBR,RVR
COMMON /MOLCON/ END,GAS,IE,I2,LAHM,MOL,OX,ZERO
COMMON /POINTS/MSUM(I3),SSUM(I3),CPA(I3),DLVT(I3),DLVPT(I3)

00101 10
00101 20
00101 30
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DATE 101500

OUT1

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00174      HEAD(1) = V(I,J)
00175      WRITE(JOUT,HEAD)
00176      60 WRITE(JOUT,HEAD)
00177      1 ENTHIN(1),FAZIN(1),RTENP(1),DENSI(1)
00178      FPC = 100./((1.0+OF1)
00179      WRITE(JOUT,20) OF1
00180      20 FORMAT(1H0.1X,4H0/F=,1A8.0X,1HPERCENT,SUC=,1A8.0X,
00181      1 1HMEQUIVALENCE RATIO=,F7.0,1X,ONDENSITY=,F8.0)
00182      IF (CF+1.0) .69,
00183      COF=0/CF
00184      WRITE(JOUT,22) COF,UCR,PER
00185      22 FORMAT(12H,OXIDIZER/COAL=,F8.0,1X,WATER/COAL=,F8.0,
00186      1 1X,5H,CARBON CONVERSION=,F8.0)
00187      60 RETURN
00188      C
00189      ENTRY OUT2
00190      C
00191      VOLUME
00192      FMT(3) = ONE
00193      IF(JMOD-VOL1,60 TO 50)
00194      CALL VARFMTVLM,NPT)
00195      WRITE(JOUT,FMT) FVLM,FB,(VLM(I), I = 1,NPT)
00196      C PREATURE
00197      50 IFLAG=0
00198      IF (CF+1.0) .52,
00199      IFLAG=1
00200      52 DO 55 I=1,NPT
00201      IF (IFLAG.EQ.0) V(I)=ATHM,PPP(I)
00202      IF (IFLAG.EQ.1) V(I)=PATHM,PPP(I)
00203      55 CONTINUE
00204      CALL VARFMTV,NPT)
00205      IF (IFLAG.EQ.0) WRITE(JOUT,FMT) FAP,FB,(V(I),J=1,NPT)
00206      IF (IFLAG.EQ.1) WRITE(JOUT,FMT) FPP,FB,(V(I),J=1,NPT)
00207      C TEMPERATURE
00208      FMT(3) = F13
00209      FMT(4) = TWO
00210      IF (IFLAG.EQ.1) 60 TO 74
00211      DO 72 J=1,NPT
00212      72 TTT(J)=TTT(J)-273.15)01.032.
00213      74 IF (IFLAG.EQ.0) WRITE(JOUT,FMT) TTM,FB,(TTT(J),J=1,NPT)
00214      IF (IFLAG.EQ.1) WRITE(JOUT,FMT) TTP,FB,(TTT(J),J=1,NPT)
00215      C ENTHALPY
00216      DO 75 I=1,NPT
00217      V(I)=HAR,HSUM(I)
00218      IF (IFLAG.EQ.1) V(I)=VII)01.0
00219      75 CONTINUE
00220      IF (IFLAG.EQ.0) WRITE(JOUT,FMT) FM,FB,(V(I),J=1,NPT)
00221      IF (IFLAG.EQ.1) WRITE(JOUT,FMT) FMM,FB,(V(I),J=1,NPT)
00222      C ENTROPY
00223      FMT(4) = FOUR
00224      DO 76 I = 1,NPT
00225      V(I) = HBAR,SSUM(I)
00226      IF (IFLAG.EQ.0) WRITE(JOUT,FMT) FS,FB,(V(I),J=1,NPT)
00227      IF (IFLAG.EQ.1) WRITE(JOUT,FMT) FSS,FB,(V(I),J=1,NPT)
00228      C DENSITY
00229      DO 70 I = 1,NPT
00230      IF (VLM(I).GT.0) V(I)=1./VLM(I)
00231      IF (IFLAG.EQ.1) V(I)=VII)02206./35.31
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OUT 1

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00400 118* 70 CONTINUE
00402 119* IF (IFLAG.EQ.0) WRITE (JOUT,1) (V(I),J=1,NPT)
00451 120* 1 FORMAT (1X,14HO DENSITY G/CC ,1P13E9.3)
00452 121* IF (IFLAG.EQ.1) WRITE (JOUT,2) (V(I),J=1,NPT)
00461 122* 2 FORMAT (1X,14HO DENSITY L/F*3 ,1P13E9.3)
00462 123* WRITE (JOUT,AD1)
00464 124* 80 FORMAT (1X,1)
00464 125* C MOLECULAR WEIGHT
00465 126* WRITE (JOUT,FMT) FM,FB,(WM(J),J=1,NPT)
00465 127* C (DLV/DLP)T
00475 128* IF (EQL) WRITE (JOUT,FMT) F,FB,(DLVPT(J),J=1,NPT)
00475 129* C (DLV/DLP)R
00506 130* IF (EQL) WRITE (JOUT,FMT) FV,FB,(DLVTP(J),J=1,NPT)
00506 131* C HEAT CAPACITY
00517 132* DO 85 I=1,NPT
00522 133* 85 V(I)=RBR*CPR(I)
00524 134* WRITE (JOUT,FMT) FCP,(V(I),J=1,NPT)
00529 135* C GAMMA(S)
00533 136* WRITE (JOUT,FMT) FG,FB,(GAMMA(S(J),J=1,NPT)
00533 137* C SONIC VELOCITY
00543 138* FMT(4)=TWO
00544 139* DO 95 I=1,NPT
00547 140* 95 S(VEL(I))=SORT(RBR*GAMMA(S(I),ITT(I)/NM(I))
00551 141* WRITE (JOUT,FMT) FSV,FVEL,(SONVEL(J),J=1,NPT)
00561 142* CALL MOVABS(500,50)
00562 143* CALL HOLDIT
00563 144* CALL PAGIT
00564 145* RETURN
00565 146* C
00566 147* ENTRY OUT1
00571 148* IF (CF+1.0) ,130,
00571 149* CCF=OF/CF
00572 150* WRITE (JOUT,22) CCF,MCR,PER
00577 151* 130 WRITE (JOUT,80)
00601 152* MD = 0
00601 153* C MOLE FRACTIONS (EQUILIBRIUM OR FROZEN)
00602 154* WRITE (JOUT,280)
00604 155* 280 FORMAT (15HO MOLE FRACTIONS/)
00605 156* IF (.NOT. EQL) GO TO 175
00605 157* C EQUILIBRIUM MOLE FRACTIONS
00607 158* DO 170 K=1,MS
00612 159* DO 140 I=1,NPT
00613 160* 140 V(I)=EMK(I)/TOTN(I)
00617 161* DO 150 I=1,NPT
00622 162* 150 IF (V(I) .GE. 5.0E-7) GO TO 160
00625 163* MD = 1
00626 164* GO TO 170
00627 165* 160 WRITE (JOUT,340) (SUB(K,J),J=1,3),FB,IV(I),I=1,NPT)
00642 166* 340 FORMAT (1X,3A4,A2,1P13E9.3)
00643 167* 170 CONTINUE
00643 168* C OUTPUT COMPLETE GO EXIT
00645 169* GO TO 211
00645 170* C FROZEN MOLE FRACTIONS
00646 171* J = 0
00647 172* DO 179 K=1,MS
00652 173* V(J+1)=EM(K,1)/TOTN(1)

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01013 229* DO 502 I=1,NPT 001440
01016 230* SUM=0. 001440
01017 231* DO 500 J=1,NS 001443
01022 232* IF (IUSE(J).NE.0) GO TO 500 001443
01023 233* SUM=SUM+EM(J,I)/TOTN(I) 001444
01024 234* 500 CONTINUE 001453
01027 235* CMV(I)=VM(I)*SUM 001453
01030 236* 502 CONTINUE 001461
01032 237* WRITE (JOUT,504) (CMV(I),I=1,NPT) 001461
01040 238* 504 FORMAT (1X,MIXTURE MV*,IX,13F9.5) 001477
01048 239* C LOCATE DR* ELEMENTS 001477
01049 240* DO 510 I=1,6 001477
01049 241* DO 508 J=1,NS 001510
01047 242* DO 506 K=1,3 001520
01052 243* IF (I06(I,K).NE.ISU0(J,K)) GO TO 508 001527
01054 244* 506 CONTINUE 001527
01056 245* IMX(I)=J 001527
01057 246* 50 IO 510 001531
01060 247* 508 CONTINUE 001534
01062 248* IMX(I)=0 001534
01063 249* 510 CONTINUE 001540
01065 250* DO 516 I=1,NPT 001540
01070 251* SUM=0. 001567
01071 252* DO 518 J=1,6 001573
01074 253* IJ=IMX(J) 001573
01075 254* IF (IJ.EQ.0) GO TO 514 001574
01077 255* SUM=SUM+EM(IJ,I) 001576
01100 256* 514 CONTINUE 001605
01102 257* XDP(I)=SUM/TOTN(I) 001605
01103 258* 516 CONTINUE 001612
01105 259* WRITE (JOUT,520) (XDP(I),I=1,NPT) 001612
01113 260* 520 FORMAT (1X,MF OF CDG*,5X,13F9.5) 001627
01114 261* DO 522 I=1,NPT 001627
01117 262* YDPS(I)=(385.2*XDP(I)/CMV(I))*((1./CF)*(1.+OF)) 001627
01120 263* 522 CONTINUE 001634
01122 264* WRITE (JOUT,524) (YDPS(I),I=1,NPT) 001634
01130 265* 524 FORMAT (1X,Y SAT SCF/LB*,2X,13F9.5) 001646
01131 266* L1=IMX(1) 001646
01132 267* L3=IMX(3) 001650
01133 268* L4=IMX(4) 001652
01134 269* DO 530 I=1,NPT 001662
01137 270* SUM=0. 001675
01140 271* IF (L4.NE.0) SUM=SUM+319.2*EM(L4,I)/TOTN(I) 001677
01142 272* IF (L1.NE.0) SUM=SUM+316.0*EM(L1,I)/TOTN(I) 001710
01144 273* IF (L3.NE.0) SUM=SUM+994.0*EM(L3,I)/TOTN(I) 001721
01146 274* HMVS(I)=SUM/XDP(I) 001732
01147 275* 530 CONTINUE 001737
01151 276* WRITE (JOUT,532) (HMVS(I),I=1,NPT) 001737
01157 277* 532 FORMAT (1X,HMV SAT B/SCF*,1X,13F9.2) 001760
01160 278* DO 538 I=1,NPT 001760
01163 279* EE(I)=HMVS(I)*YDPS(I)/HMV 001760
01164 280* YDP(I)=379.5*YDPS(I)/385.2 001764
01165 281* HMV0(I)=(385.2/379.5)*HMVS(I) 001770
01166 282* IF (L0.NE.0) LHMVS(I)=HMVS(I)-(1059.9*18./385.2)*(EM(L4,I)/TOTN(I)) 001773
01166 283* X /XDP(I) 001773
01170 284* LHMV(I)=LHMVS(I)*385.2/379.5 002004

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OUT1

DATE 101500

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01171 285*      DOL(I)=10000.*(1.25*HHVV/10000.+OF(CF)/(HHVS(I)*YDPS(I)))
01172 286*      530 CONTINUE
01174 287*      WRITE (JOUT,542) (EE(I),I=1,NPT)
01202 288*      542 FORMAT (1X,'EFFICIENCY',4X,13F9.5)
01203 289*      WRITE (JOUT,544) (YD(I),I=1,NPT)
01211 290*      544 FORMAT (1X,'Y DRY SEC/LB',2X,13F9.5)
01212 291*      WRITE (JOUT,546) (HHVD(I),I=1,NPT)
01220 292*      546 FORMAT (1X,'HHV DRY B/SCF',3X,13F9.2)
01221 293*      WRITE (JOUT,548) (LHVS(I),I=1,NPT)
01227 294*      548 FORMAT (1X,'LHV SAT B/SCF',3X,13F9.2)
01230 295*      WRITE (JOUT,550) (LHVD(I),I=1,NPT)
01236 296*      550 FORMAT (1X,'LHV DRY B/SCF',3X,13F9.2)
01237 297*      WRITE (JOUT,552) (DOL(I),I=1,NPT)
01245 298*      552 FORMAT (1X,'S PER MBTU',3X,13F9.2)
01246 299*      560 CONTINUE
01247 300*      RETURN
01250 301*      END

```

OUTP0137

END OF COMPILATION:

1 DIAGNOSTICS.

3H06.P

PROK

PROK

DATE 101380

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1

3PDP.LWF PROK PROK
PDP12R1 R72-16 10/15/80 13:07:27 (0.0) RI
PF0001 SPECPR PROC
0002 COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLW(150),MD(150)
0003 1,DELW(150),A(15,150),SUB(150,3),IUSE(150),TEMP(90,2),SLN(150)
0004 DATA MSPP1/151/
0005 END

END PDP ERRORS : NONE

3H06.P REACT

REACT

BF2R,S REACT,REACT
MSA E3 -10/18/80-13:07:28 (31.)

SUBROUTINE R_EACT ENTRY POINT 001077

STORAGE USED: CODE(1) 001111; DATA(0) 000367; BLANK COMMON(2) 000000

COMMON BLOCKS:

0003 HOLCON 000010
0004 MISC 001701
0005 IMOX 000041
0006 CCC 000003
0007 CFUEL 000004

EXTERNAL REFERENCES (BLOCK, NAME)

0010 OUT
0011 RNCDS
0012 MOVARS
0013 HOLDOUT
0014 PAGIT
0015 MREWS
0016 MRBUS
0017 NI028
0020 NI015
0021 MWDUS
0022 MERR35

STORAGE ASSIGNMENT (BLOCK, TYPE, RELATIVE LOCATION, NAME)

0001	000327	1011	0001	000001	132E	0001	000011	1438	0001	000072	14L	0001	000074	20L
0001	000463	200L	0001	000521	204L	0001	000106	2046	0001	000557	210L	0001	000318	212F
0001	000566	214L	0001	000736	210L	0001	000740	220L	0001	001002	222L	0001	001005	224L
0001	001022	224L	0001	001042	229L	0001	001056	230L	0001	000146	232E	0001	000233	2676
0001	000243	2756	0000	000301	30F	0001	000256	3046	0001	000300	3176	0001	000377	3426
0001	000226	371L	0001	000512	4006	0001	000834	4148	0001	000554	4306	0001	000617	4476
0001	000270	45L	0001	000275	46L	0001	000642	4608	0001	000712	4736	0001	000311	50L
0001	000766	5106	0001	000771	5136	0001	001012	5316	0001	001033	5436	0001	001046	5526
0001	000042	6L	0004	R 000640	AM	0004	000705	AM1	0004	R 001070	ANAME	0004	R 001135	ANUM
0004	R 000004	ATOM	0004	000514	BO	0004	R 000545	BOP	0005	000036	CALCH	0007	R 000000	CF
0005	000001	CONV8	0004	000706	CPRI	0004	000634	CPSUM	0004	R 000654	DATA	0006	000002	DEMAND
0004	R 001560	DENS	0003	000000	END	0004	001700	ENLSAV	0004	000000	ENW	0004	001676	ENML
0004	001677	ENSAVE	0004	R 001414	ENTH	0004	000636	EQRAT	0004	R 001445	F4Z	0004	I 001527	FOX
0003	000001	GAS	0006	000000	GRAPH	0007	R 000001	MHV	0005	000003	HP	0004	R 000642	MPP
0004	000637	HSUB0	0000	I 000262	I	0005	I 000030	IC	0005	000000	IDEBUG	0003	000002	IE
0005	000018	IMAT	0000	000344	INJPS	0000	I 000271	IO	0005	000023	IONS	0000	I 000235	IOUT
0005	000021	IP	0005	000037	IQSAVE	0005	000016	IQ1	0005	000005	ISV	0005	000034	IT
0003	I 000003	IZERO	0000	I 000266	J	0000	I 000275	JJ	0005	000026	JL10	0006	I 000001	JOUT
0005	000025	JSOL	0005	000031	JS1	0000	I 000265	M	0005	000014	KMAT	0005	I 000012	L
0003	I 000004	LANK	0000	I 000145	LINE1	0000	I 000172	LINE2	0000	I 000215	LINE3	0004	I 000463	LLMT
0000	I 000032	LLMTS	0005	000040	LSAVE	0003	I 000005	MOL	0000	I 000272	MOLE	0005	L 000006	MOLES

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0000 I 000270 M
0005 L 000022 NEWR
0005 000017 NOF
0005 000013 MS
0003 I 000006 OX
0003 I 000003 PP
0004 R 001976 RTEMP
0004 000003 SO
0004 000031 YMD
0005 000012 VOL

0000 I 000707 NAME
0000 I 000267 MFUEL
0005 I 000020 MWT
0005 000018 RT
0004 001644 OXF
0004 R 000044 RH
0004 R 000063 SRP
0004 000032 THIGH
0005 000002 TP
0004 R 000650 VPLS

0000 I 000273 MAST
0000 000035 MFZ
0005 000007 NP
0000 I 000263 N3
0000 R 000276 PCWT
0000 001611 R40P
0004 000033 SHOCK
0005 001643 TLM
0004 000002 TT
0007 R 000002 MCR

0000 I 000024 MC
0000 I 000000 NLS
0005 000000 MPT
0000 000011 NB
0004 R 001363 PECWT
0004 R 000274 RM
0005 000004 SP
0004 000630 TLOW
0004 000001 V
0004 R 000001 VM
0003 I 000007 ZERO
    
```

```

00101 SUBROUTINE REACT
00101 C
00103 COMMON /MOLCON/ END,GAS,IE,IZERO,LANK,MOL,OX,ZERO
00103 COMMON /MISC/ LHM,SUM,II,SG,ATOMIS,IOL,LLMT(25),BOL(25),
00104 BOP(25,2),TM,TLOW,THID,THIGH,PP,CPSUM,OF,EQRAT,
00104 HSUBO,AM(2),MPP(2),RM(2),VMIN(2),VPLS(2),MP(2),
00104 DATA(25),AM1,CPR1,NAME(25,6),AMUM(25,6),PECWT(25),
00104 ENTH(25),FAZI(25),RTEMP(25),FOX(25),DENS(25),PMOP,
00104 RMW(25),TLM,OXF(26),CNML,ENSAVE,EM,SAV
00105 COMMON /INDEX/ IDEXB,CONVE,IP,MP,SP,ISV,MOLES,MP,MT,MPI,L,MS,
00105 KMAT THAT,IQ1,NOF,MONIT,IP,NEWR,IONS,NC,JSL,IQ,
00105 MREAC,IC,JSL,VOL,SHOCK,IT,MFZ,CALCH,IOSAVE,LSAVE
00105 C
00105 COMMON /CCG/ GRAPH,JOUT,DEMAND
00105 C
00105 COMMON /CFUEL/CF,MHVV,MCR,PER
00105 DATA NLS/D/
00105 DIMENSION ANAME(25,6),V(25),LLMTS(25),SBOP(25,2)
00105 EQUIVALENCE (NAME,ANAME)
00105 INTEGER FOX,OX,ZERO
00105 LOGICAL MOLES,NEWR
00105 DIMENSION LINE1(21),LINE2(19),LINE3(16)
00105 DIMENSION IOUT(21)
00105 DATA (LINE1(I),I=1,21),INDEX,4*
00105 X REACTA,MT(1),3*
00105 X EL WT,*,*,MOL,E ENT,HALPY,*,*,R,*,
00105 X PHA,SE TE,MP,K*,*,FUEL,*,*,DENS,ITY */
00105 DATA (LINE2(I),I=1,19),10*
00105 X N,O MOLE,S*,*,INT,*,
00105 X ENER6,*,*,2*,*,OXID,*/
00105 DATA (LINE3(I),I=1,16),8*
00105 X *,*,IND,ICATES,*,*,ENTHA,*,*,LPY TO,*,*,BE CA,*,
00105 X LCLULAT,*,*,ED */
00105 C
00105 DATA N3/8/,NB/12/
00105 C
00105 DO 8 K = 1,2
00105 MP(K)=0.
00105 HPP(K)=0.
00105 RH(K)=0.
00105 VPLS(K)=0.
    
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REACT

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00140 430 VMIN(K)=0. 000006
00141 440 AMIN(K)=0. 000007
00142 450 DO 8 J=1,25 000013
00143 460 LLMT(J)=0 000013
00144 470 8 BOP(J,M) = 0.0 000013
00151 480 MFUEL = 0 000017
00152 490 N=1 000020
00153 500 C WRITE REACTANT HEADER 000020
00154 510 CALL GOUTLINE1,126) 000022
00155 520 CALL GOUTLINE2,119) 000026
00156 530 L=1 070032
00157 540 IQ=13 000034
00158 550 C READ REACTANTS 000034
00159 560 REMIND IO 000036
00160 570 6 READ (IO) NREAC,CF 000042
00161 580 10 IF (IO.EQ.NR) GO TO 20 000047
00162 590 IF (CF,1.0) ,18, 000052
00171 600 REMIND IC 000056
00172 610 READ (NR) NREAC,CF,MHVV,CH,CR,PER 000060
00173 620 18 IF (NREAC.EQ.0) GO TO 20 000072
00174 630 20 IF CONTINUE 000074
00175 640 READ (IO) (NAME(M,I),ANUM(M,I),I=1,5),PECT(M),MOLE,ENTH(M), 000074
00176 650 X NAME(M,6),ANUM(M,6),FAZ(M), 000074
00177 660 X RTEMP(M),FOX(M),DENSM 000074
00178 670 NAST=1H 000124
00179 680 IF (NAME(M,6).EQ.2HOD) NAST=1H 000127
00180 690 ENCODE (10,10UT) N,(NAME(M,J),ANUM(M,J),J=1,5),PECT(M),MOLE, 000135
00181 700 X ENTH(M),NAST,FAZ(M),RTEMP(M),FOX(M),DENSM 000135
00182 710 CALL GOUT(10UT,126) 000164
00183 720 30 FORMAT (11,12,15,12,5,12,5,9,2X),F10.6,2X,A1,F13.0,A1,3X,A1,F12.3, 000170
00184 730 X 3X,A1,F12.5,1X) 000170
00185 740 IFIL.EQ.0160 TO 20 000170
00186 750 IF (MOLE.EQ.0) MOLES = .TRUE. 000172
00187 760 IF OXIDANT, K = 1: IF FUEL, K = 2. 000172
00188 770 IF(FOX(M).EQ.2E0) FOX(M)=OX 000177
00189 780 IF (SPEC(M) .LE. 0.0) PECT(M) = 1.0 000205
00190 790 K = 1 000213
00191 800 IF(FOX(M).EQ.OX) GO TO 37 000215
00192 810 K = 2 000221
00193 820 MFUEL = MFUEL*1 000223
00194 830 37 DO 38 J=1,25 000226
00195 840 38 DATA(J) = 0.0 000231
00196 850 RH=0. 000234
00197 860 DO 100 JJ=1,6 000243
00198 870 IF (ANUM(M,JJ) .LE. 0.0) GO TO 101 000243
00199 880 IF (NAME(M,JJ) .EQ. 2E0) NAME(M,JJ) = OX 000246
00200 890 DO 91 J=1,15 000254
00201 900 I = J 000256
00202 910 IF(LLMT(J).EQ.0) GO TO 95 000256
00203 920 91 IF (NAME(M,JJ) .EQ. LLMT(J)) GO TO 96 000260
00204 930 95 L = I 000262
00205 940 LLMT(J)=NAME(M,JJ) 000270
00206 950 DO 98 I = 1,101 000272
00207 960 98 IF (ATOM(I,1) .EQ. ANAME(M,JJ)) GO TO 50 000300
00208 970 L=0 000306
00209 980 GO TO 20 000307

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ORIGINAL PAGE IS
OF POOR QUALITY

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00326 990 50 RM = RM + ANUMIN*JJ*ATOM(2,I)
00327 1000 V(I,J) = ATOM(I,J,I)
00330 101 100 DATA(J) = ANUMIN(JJ)
00332 102 101 PCMT=PCMT(N)
00333 103 IF(MOLES) PCMT=PCMT*RM
00335 104 MP(K)=MP(K) + PCMT
00336 105 IF (NAME(N,6).NE.IZERO) HPP(K)=HPP(K)+ENTHMIN*PCMT/RM
00340 106 AM(K)=AM(K)+PCMT/RM
00341 107 DO 110 J=1,L
00344 108 110 ROP(J,K) = DATA(J)*PCMT/RM + BOP(J,K)
00346 109 IF (DEMS(N) .GT. 0.0) RH(K) = RH(K) + PCMT/DEMS(N)
00350 110 RM(N) = RM
00351 111 M = N+1
00352 112 IF (M.EQ.26) GO TO 200
00354 113 IF (I.O.EQ.N3.AND.N-1.EQ.NREAC) GO TO 200
00356 114 IF (I.O.EQ.NB.AND.N-1.EQ.NM1*NEAC) GO TO 200
00360 115 GO TO 20
00361 116 200 NM1=M-1
00362 117 IF (I.O.EQ.NB) GO TO 204
00364 118 IO=NB
00365 119 REWIND IO
00366 120 READ (IO) NREAC,CF,MHVV,UCR,PER
00375 121 IF (NREAC.EQ.0) GO TO 204
00377 122 DO 202 I=1,N
00402 123 READ (IO) NDUHMY
00405 124 202 CONTINUE
00407 125 GO TO 6
00410 126 204 NREAC=NM1
00411 127 IF(FUEL-6T-0) GO TO 210
00413 128 C 100 PERCENT OXIDANT, CALL REACTANTS_FUEL
00415 129 DO 205 N=1,NREAC
00416 130 205 FOX(N) = LANK
00420 131 RH(2) = RH(1)
00421 132 RH(1) = 0.
00422 133 WP(2) = WP(1)
00423 134 MP(1) = 0.
00424 135 HPP(2) = HPP(1)
00425 136 AM(2) = AM(1)
00426 137 AM(1) = 0.
00427 138 DO 208 J=1,L
00432 139 208 BOP(J,2) = BOP(J,1)
00434 140 210 IF (L.NE.0) GO TO 214
00436 141 WRITE (JOUT,212)
00440 142 212 FORMAT ('0','ERROR IN REACTANT DATA')
00441 143 214 CALL GOUT(' ',1)
00442 144 CALL GOUT(LINE3,56)
00443 145 CALL MOVABS(500,50)
00444 146 CALL HOLDIT
00445 147 CALL PAGIT
00446 148 DO 220 K=1,2
00451 149 IF (WP(K) .LE. 0.0) GO TO 220
00453 150 HPP(K)=HPP(W)/MP(K)
00454 151 AM(K) = WP(K)/AM(K)
00455 152 IF (RH(K) .GT. 0.0) RH(K) = WP(K)/RH(K)
00457 153 DO 215 J=1,L
00462 154 BOP(J,M)=BOP(J,K)/WP(K)
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00463 1550 IF(V(J),LT 9,VMIN(K)=VMIN(K)+BOP(J,K)*V(J) 000669
00465 1560 215 IF(V(J),.6V,0.0) VPLS(K)=VPLS(K)+BOP(J,K)*V(J) 000673
00470 1570 IF(MOLE) GO TO 220 000705
00472 1580 DO 210 N=1,NREAC 000712
00475 1590 IF((F(N)*EQ-OR-AND-K.EQ-2).OR.(FOX(N)*WE-OR-AND-K.EQ-1))GO TO 218 000712
00477 1600 PECHT(N)=PECHT(N)/VPLS(N) 000732
00500 1610 218 CONTINUE 000742
00502 1620 220 CONTINUE 000742
00504 1630 NEUR=.TRUE. 000742
00508 1640 C ARE ELEMENTS SAME AS FOR LAST SET OF REACTANTS, IF SO, NEUR=.FALSE. 4/23/70 000744
00509 1650 IF (L.NE. NLS .OR. MONIT .PE. 0) GO TO 226 000766
00507 1660 DO 224 I=1,NLS 000771
00512 1670 DO 222 J=1,L 000771
00515 1680 IF(LLMT(J).NE.LLMTS(I)) GO TO 222 000774
00517 1690 SBOP(I,1)=BOP(J,1) 000776
00520 1700 SBOP(I,2)=BOP(J,2) 001000
00521 1710 GO TO 224 001003
00522 1720 222 CONTINUE 001006
00524 1730 GO TO 226 001012
00525 1740 224 CONTINUE 001012
00527 1750 NEUR=.FALSE. 001012
00530 1760 DO 225 I=1,L 001012
00533 1770 LLMT(I)=LLMTS(I) 001012
00534 1780 BOP(I,1)=SBOP(I,1) 001013
00535 1790 225 BOP(I,2)=SBOP(I,2) 001013
00537 1800 226 NLS=L 001020
00540 1810 REWIND 4 001022
00541 1820 DO 228 I=1,L 001023
00542 1830 SBOP(I,1)=BOP(I,1) 001026
00543 1840 SBOP(I,2)=BOP(I,2) 001031
00546 1850 228 LLMTS(I)=LLMT(I) 001034
00547 1860 229 DO 230 N=1,NREAC 001036
00551 1870 IF (DENS(N).GT. 0.0) GO TO 230 001042
00554 1880 RH(2)=0. 001046
00556 1890 RH(1)=0. 001050
00557 1900 RETURN 001051
00560 1910 230 CONTINUE 001052
00561 1920 RETURN 001057
00563 1930 001057
00564 1940 001110

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ACTM0111

END OF COMPILATION: NO DIAGNOSTICS.

AMOG.P RTOUT

AFOR.S RRTOUT, RRTOUT
MSA 53 -10/15/80-13:07:33 (12.1)

SUBROUTINE RRTOUT ENTRY POINT 000532

STORAGE USED: CODE(1) 000581; DATA(1) 000122; BLANK COMMON(2) 000000

COMMON BLOCKS:

0003 COMETS 000004
0004 POINTS 000335
0005 SPECIES 017104
0006 INDX 000001
0007 PERF 000164
0010 OUPY 000073
0011 CCC 000003
0012 CFUEL 000001

EXTERNAL REFERENCES (BLOCK, NAME),

0013 MOVARS
0014 OUT1
0015 VARFMT
0016 OUT2
0017 GAMEFF
0020 OUT3
0021 OUT4
0022 MOVARS
0023 MIO2S
0024 MIO1S
0025 SQRT
0026 MIO3S
0027 NERR3S

STORAGE ASSIGNMENT (BLOCK, TYPE, RELATIVE LOCATION, NAME)

0001	000063	1466	0000	000066	150F	0001	000074	1546	0001	000121	1706	0001	000150	2006					
0001	000202	200L	0000	000075	208F	0001	000422	220L	0001	000235	222G	0001	000263	2366					
0001	000316	254G	0001	000340	2666	0001	000350	2746	0001	000366	3056	0001	000511	312L					
0001	000416	321G	0001	000427	3266	0001	000445	3376	0001	000466	3506	0001	000505	3606					
0000	000006	37F	0000	000027	387F	0000	000056	40F	0001	000520	400L	0000	000047	737F					
0005	011052	A	0007	P	030150	AFAT	0007	R	000133	APP	0003	R	000000	ATMM					
0006	000036	CALCH	0012	R	030000	CF	0005	000000	COEF	0006	000001	CONVG	0000	R	000002	AV			
0000	R	000005	CS1R	0005	010624	DELM	0011	000002	DEMANO	0004	000064	DLVPT	0004	000032	CPR				
0005	00312	EW	0005	010150	EPLM	0007	L	000165	EOL	0010	R	000002	FA	0010	000003	FAP			
0010	R	000005	FR	0010	R	000006	FC	0010	000007	FCP	0010	R	000012	FCST	0010	R	000014	FCV	
0010	R	000015	FG	0010	R	000017	FGE	0010	R	000020	FGV	0010	R	000021	FM	0010	R	000023	FI
0010	R	000025	FIV	0010	000027	FH	0010	R	000031	FMT	0010	R	000050	FM	0010	R	000052	FOUR	
0010	R	000053	FP	0010	000054	FS	0010	000056	FSV	0010	000057	FT	0010	000061	FTM	0004	R	000101	GAMPAS
0010	000063	FV	0010	R	000065	FVEL	0010	R	000001	F13	0010	R	000000	F9X	0005	R	010376	HO	
0003	R	000001	GPLET	0011	000000	GRAPH	0006	000003	HP	0004	R	000000	HSUM	0007	000105	IMJP4			
0000	I	000004	I	0006	000030	IC	0006	000000	IDERUS	0006	000015	IMAT							

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0006 I 000023 IONS      0006 000021 IP      0006 000037 ICSAVE      0006 000016 IOUT      0006 000005 ISV
0006 I 000034 IT        0006 016266 IUSE      0006 000027 JLIO      0006 000001 JOUT      0006 000025 JSOL
0006 000031 JSI        0006 000003 K          0006 000019 KMAT      0006 000000 LSAVE      0006 000006 MOLES
0006 000030 MC          0006 000022 MEWR      0006 000035 MP2      0006 000012 MLM      0006 000017 MOF
0006 000030 MORIT      0006 000007 MP          0006 000011 MP2      0006 000027 MPEAC      0006 000013 MS
0006 I 000000 MSPL      0006 000010 MT          0006 000047 ONE      0006 000016 P          0006 000002 PATH
0007 000000 PCP        0006 R 000021 PPP      0006 000003 R8R      0006 000004 RBR      0006 000005 RVR
0006 000047 PIM        0006 000033 SHOCK      0006 016660 SLN      0006 R 000025 SONVEL      0006 000000 SP
0006 R 000150 T        0006 000001 TEM      0006 016514 TEMP      0006 000101 SUBAR      0006 000116 SUPAR
0006 000002 TP        0006 R 000266 TTY      0006 000071 TWO      0006 000070 THREE      0006 000320 TOTM
0006 000101 VLM        0006 R 000032 VMOE      0006 000032 VOL      0006 R 000071 VACI      0006 000072 ZERO

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00101 10 SUBROUTINE ARTOUT (IGAM)
00101 20 C
00101 30 C ROCKET PERFORMANCE PARAMETERS
00101 40 C
00101 50 COMMON /CONSTS/ ATNM,GMET,PATH,RBAR,RBR,RVR
00101 60 COMMON/POINTS/MSUM(13),SSUM(13),CPR(13),OLVTP(13),OLVPT(13)
00101 70 1,GMAT(13),P(26),V(13),PP(13),WM(13),SONVEL(13),TTY(13)
00101 80 2,ALH(13),JL(13),JLIM(13)
00101 90 C
00101 100 COMMON/SPECES/COEFF(7,150),S(150),EM(150,13),MLM(150),MO(150)
00101 110 C
00101 120 COMMON/INDEX/ IOEBUS,CONVE,TP,MP,SP,ISV,MOLES,MP,MT,MPT,MLM,MS,
00101 130 KMAT,IMAT,QI,MOF,NOMIT,IP,MEWR,IONS,MC,JSOL,JLIO,
00101 140 MPEAC,IC,JL,VOL,SHOCK,IL,MZ,CALCM,ISAVE,ISAVE
00101 150 COMMON /PERF/ PCPI(20),VMOC(13),SPIN(13),VACI(13),SUBAR(13),
00101 160 SUPAR(13),AP(13),AEAT(13),EOL
00101 170 COMMON /OUT/ F9X,F13,FA,FAP(2),FB,FC,FCP(3),FCST(2),FCU,FG(2),
00101 180 FGE,F8V,FM(2),F(12),FIV(2),FM(2),FMT(18),FM(2),FOUR,
00101 190 FP,F5(2),FSV,FT(2),FTN(2),FVEL(2),ONE,THREE,
00101 200 TWO,ZERO
00101 210 C
00101 220 COMMON /CCC/ GRAPH,JOUT,DEMAND
00101 230 C
00101 240 COMMON /CFUEL/CF
00101 250 LOGICAL EOL
00101 260 CALL MOVABS(500,50)
00101 270 IF(EOL) WRITE(JOUT,37)
00101 280 37 FORMAT(1M/2X,8HTHEORETICAL ROCKET PERFORMANCE ASSUMING EQUILIBRIUM COMPOSITION DURING EXPANSION
00101 290 11UM COMPOSITION DURING EXPANSION
00101 300 IF (.NOT.EOL) WRITE(JOUT,38)
00101 310 38 FORMAT(1M/2X,7HTHEORETICAL ROCKET PERFORMANCE ASSUMING FROZEN COMPOSITION DURING EXPANSION
00101 320 10POSITION DURING EXPANSION
00101 330 IF(TTY(1),EQ.TTY(1)) WRITE(JOUT,737)
00101 340 737 FORMAT (5X,28HAT AN ASSIGNED TEMPERATURE
00101 350 TEM = PATHOPPP(1)
00101 360 AV = ATNMOPPP(1)
00101 370 WRITE(JOUT,40) TEM,AV
00101 380 40 FORMAT (5H PC =,F10.3,7H PSIA =,1PE13.6,7H N/MOP2)
00101 390 CALL OUT1
00101 400 K = MPT - 2

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00145 410 DO 20 I = 1,K
00150 420 V(I) = QMEX(I)
00152 430 WRITE(JOUT,ISO) (V(I), I = 1,K)
00160 440 FORMAT (1MO,6X,10HCHAMBER THROTT,11(5X,4N1))
00162 450 C PRESSURE RATIOS
00164 460 FMT(1) = ONE
00166 470 CALL VARFMT (APP,MPT)
00168 480 WRITE(JOUT,FMT) FV,FB,FB,(APP(I), I = 1,MPT)
00170 490 CALL OUT2
00172 500 IF (MPT .LT. 2) GO TO 312
00174 510 DO 202 K=2,MPT
00176 520 SPIN(K) = SBRI2,QBRR,MSUM(I,1 - MSUM(I))/GMEI
00178 530 C A (A/V) IN UNITS OF SEC/ATM
00180 540 AV = BROTT(I)/(IPPM(K)*M)*SPIN(K)*GMEI**2
00182 550 IF (M*2160 TO 200
00184 560 CSTR = GMEI*AV*PPPI(1)
00186 570 ACAT(2) = 1.
00188 580 200 VACI(K) = SPIN(K)*APP*AK*IAAM
00190 590 IF (SONVEL(I) .GT. 0.0) VMOC(K) = GMEI*SPIN(K)/SONVEL(K)
00192 600 202 V(K) = GMEI*SPIN(K)
00194 610 V(I) = 0.0
00196 620 WRITE(JOUT,FMT) FV,FVEL,(V(I), I = 1,MPT)
00198 630 C MACH NUMBER
00200 640 FMT(4) = FOUR
00202 650 VMOC(1) = 0.
00204 660 IF (GAMMA(2) .LE. 0.0) VMOC(2) = 0.0
00206 670 WRITE(JOUT,FMT) FM,FB,(VMOC(I), I = 1,MPT)
00208 680 200 FORMAT (1M)
00210 690 C AREA RATIO
00212 700 CALL VARFMT (AET,MPT)
00214 710 FMT(3) = F9X
00216 720 WRITE(JOUT,FMT) FA,FB,FB,(AET(I), I = 2,MPT)
00218 730 C
00220 740 CSTAR
00222 750 FMT(4) = F13
00224 760 FMT(5) = TWO
00226 770 WRITE(JOUT,FMT) FCST,FB,FCSTR, I = 2,MPT)
00228 780 C CF - THRUST COEFFICIENT
00230 790 FMT(5) = FOUR
00232 800 DO 212 I=2,MPT
00234 810 212 V(I) = GMEI*SPIN(I)/CSTR
00236 820 WRITE(JOUT,FMT) FC,FB,FB,(V(I), I = 2,MPT)
00238 830 IF (IGAM .EQ. 0) GO TO 220
00240 840 C EFFECTIVE GAMMA
00242 850 CALL GAMEFF (V,GAMMA,APP,MPT,MO)
00244 860 WRITE(JOUT,FMT) FG(1),FGE,FR,(MO(I), I = 2,MPT)
00246 870 C VACUUM THRUST COEFFICIENT
00248 880 220 DO 230 I = 2,MPT
00250 890 230 V(I) = GMEI*VACI(I)/CSTR
00252 900 WRITE(JOUT,FMT) FCV,FB,FB,(V(I), I = 2,MPT)
00254 910 C VACUUM IMPULSE
00256 920 FMT(5) = THREE
00258 930 WRITE(JOUT,FMT) FIV,FB,(VACI(I), I = 2,MPT)
00260 940 C SPECIFIC IMPULSE
00262 950 WRITE(JOUT,FMT) FI,FB,(SPIN(I), I = 2,MPT)
00264 960 C FROZEN MOLE FRACTION OUTPUT MOVED TO SURPOUTTIME OUT3
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DATE 101500

RETOUR

00364	970	312 CALL OUT3	000511
00365	980	IF (CF+1.0) .000.	000512
00370	990	CALL OUT4	000515
00371	1000	400 CONTINUE	000520
00372	1010	RETURN	000520
00373	1020	END	000520

END OF COMPILATION: NO DIAGNOSTICS.

ANDG.P ROCEET

3FOR,S ROCKET,ROCKET
HSA E3 -10/15/80-13:07:36 (10.)

SJ BROUTINE ROCKET ENTRY POINT 001310

STORAGE USED: CODE(1) 001317; DATA(0) 000231; BLANK COMMON(2) 000000

COMMON BLOCKS:

0003 COMSTS 000006
0004 POINTS 000335
0005 MISC 001701
0006 INDX 000041
0007 PERF 000166
0010 CCC 000003

EXTERNAL REFERENCES (BLOCK, NAME)

0011 NEWOF
0012 FROZEN
0013 EQLBRM
0014 RKTOUT
0015 SAVE
0016 MUDUS
0017 NIQZS
0020 WRNLS
0021 MNMLS
0022 XPRR
0023 AL06
0024 EXP
0025 XPRR
0026 SORT
0027 NERR3S

STORAGE ASSIGNMENT (BLOCK, TYPE, RELATIVE LOCATION, NAME)

0001	000013	1256	0001	000162	1332L	0001	000035	1846	0001	000054	1566	0000	000104	1811F							
0001	000302	19AL	0001	000420	192L	0000	000101	194F	0001	000261	195L	0001	000126	2036							
0000	000065	302F	0001	000026	303L	0001	000045	306L	0001	000103	321L	0001	000122	322L							
0001	000153	331L	0001	000160	332L	0001	000175	333L	0001	000213	334L	0001	000610	799L							
0001	000536	800L	0001	000763	802L	0001	000640	805L	0001	000703	809L	0001	000653	810L							
0001	001007	820L	0000	000125	821F	0001	001015	830L	0001	001043	834L	0001	001053	835L							
0001	001055	859L	0001	001061	860L	0000	000137	862F	0000	000166	865F	0001	001121	870L							
0001	001135	880L	0001	000457	899L	0001	000477	900L	0000	000073	923F	0001	000416	925L							
0001	001171	990L	0001	001232	997L	0001	001264	999L	0007	R	000150	AEAT	0000	R	000037	AEATL					
0005	000640	AM	0005	000705	AM1	0005	001135	ANUM	0007	R	000133	APP	0000	R	000035	APPL					
0000	R	000033	ARATIO	0000	L	000005	AREA	0000	D	000001	ASQ	0003	000000	ATMN	0005	000004	ATOM				
0000	R	000030	AWT	0005	000514	BO	0005	000545	BOP	0006	000036	CALCH	0006	000001	COMV6	0005	000001	COMV6			
0004	R	000032	CPR	0000	R	000023	CPRF	0005	000706	CPR1	0005	R	000634	CPSUM	0005	000654	DATA	0005	000654	DATA	
0010	000002	DEMAND	0005	001560	DENS	0000	R	000026	DM	0000	R	000032	DLMP	0000	R	000040	DLNPE	0000	R	000040	DLNPE
0000	R	000027	DLT	0004	000064	DLVPT	0004	R	000047	DLVTF	0000	R	000034	ELN	0005	001700	ENLSAV	0005	001700	ENLSAV	
0005	R	000000	ENH	0005	001676	ENML	0005	001677	ENSAVE	0005	001414	ENTH	0007	L	000165	EQL	0007	L	000165	EQL	

ROCKET

DATE 101580

PAGE

2

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0005 000636 EORAT      0005 001445 FAZ      0005 001527 FOX      0000 L 000006 FROZ      0004 R 000101 GAMMAS
0003 000001 GMEY      0000 000000 GRAPH      0006 L 000003 HP      0005 000642 HPP      0005 000637 HSUBQ
0004 R 000000 HSUM      0000 I 000012 I      0006 000030 IC      0000 I 000000 ICASE      0006 I 000000 IORUG
0000 I 000011 IGAM      0006 000015 IMAT      0000 000219 INJPS      0000 I 000016 IOF      0006 000023 IOMS
0000 I 000021 IP      0000 I 000022 IPP      0006 000037 IOSAVE      0006 000016 IOI      0000 I 000020 ISUR
0000 I 000021 ISUP      0006 I 000005 ISV      0006 I 00003A IT      0000 I 000017 ITMUM      0000 I 000026 ITRAT
0006 000026 JLIO      0000 I 000001 JOUT      0006 I 000025 JSOL      0006 000031 JSI      0006 000014 KMAT
0005 000463 LLMT      0006 000040 LSARE      0006 000006 MOLES      0005 000707 NAME      0006 000024 NC
0006 000022 MEUR      0006 I 000035 MFZ      0006 000012 MLM      0006 I 000017 NOF      0006 000020 NOMIT
0006 I 000007 NP      0000 I 000013 NPP      0006 I 000011 NPT      0006 000027 MPEAC      0006 000013 NS
0000 I 000014 NSUB      0000 I 000015 NSUP      0006 I 000010 NT      0005 R 000635 OF      0005 R 001644 OXF
0004 R 000116 P      0003 000002 PATM      0007 R 000000 PCP      0000 R 000031 PCPLI      0005 001361 PECUT
0005 R 000633 PP      0004 R 000217 PPP      0003 000003 RBR      0003 R 000004 RBR      0005 000644 RH
0005 001611 RHOP      0000 000411 RKTMP      0005 001612 RMW      0005 000005 RVR      0003 000005 RVR
0000 L 000007 SEQL      0006 000033 SHOCK      0004 000251 SONVEL      0006 L 000004 SP      0007 000047 SPIM
0004 R 000015 SSUM      0007 R 000101 SUBAR      0005 000001 SUMM      0007 R 000116 SUPAR      0005 R 000003 SO
0004 R 000150 T      0000 L 000010 THI      0005 000632 THIGH      0005 001643 TLM      0005 000630 TLOW
0005 000927 TH      0000 R 000024 TMELI      0005 000621 TRIN      0000 R 000036 TOL      0004 000320 TOTM
0006 L 000002 TP      0005 R 000002 TT      0004 R 000266 TTT      0000 D 000003 USQ      0004 000202 V
0007 000064 VACT      0004 000033 VLM      0005 000646 VMIM      0007 000032 VMOC      0006 000032 VOL
0005 000650 VPLS      0004 R 000234 VM      0005 000652 VP

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ORIGINAL PAGE 1
OF FOUR QUALITY

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00101 1* C SUBROUTINE ROCKET      ROCK0002      000000
00101 2* C      ROCK0001      000000
00101 3* C ROCKET PERFORMANCE      ROCK0000*      000000
00101 4* C      /CONSTS/      000000
00103 5* COMMON /CONSTS/ ATN,GMEI,PAIM,RBAR,RBAR,RBAR      /CONSTS/      000000
COMMON/POINTS/MSUM(13),SSUM(13),CPR(13),OLVTP(13),OLVPT(13)      000000
1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),VM(13),SONVEL(13),TTT(13)      000000
2 ,VLM(13),TOTM(13)      000000
COMMON /MISC/ ENN,SUMM,TI,SO,ATON(3,101),LLMT(25),BOI(25),      000000
BOI(25,2),TM,TLOW,THID,THIGH,PP,CP,SUM,OF,EORAT,      000000
HSUBO,AM(2),HPP(2),RM(2),VM(2),VPLS(2),WP(2),      000000
DATA(25),AMI,CPR1,NAME(25,6),ANUM(25,6),PECUT(25),      000000
EMTH(25),FAZ(25),RYEMP(25),FOX(25),OEMS(25),RHOP,      000000
RMW(25),TLM,OXF(26),ENML,ENSARE,ENLSAV      000000
COMMON /INDX/ IDEBUG,CONVG,TP,HP,SP,ISV,MOLES,NP,NT,NPT,MLM,NS,      000000
IMAT,IMAT,IOI,NOF,NOMIT,IP,MEUR,IONS,NC,JSOL,JILO,      000000
NREAC,IC,J51,VOL,SHOCK,II,NFZ,CALCH,IQSARE,LSAVE      000000
COMMON /PERF/ PCPI(26),VMOC(13),SPIM(13),VACI(13),SUBAR(13),      000000
SUPAR(13),APP(13),AEAT(13),EQL      000000
1      /PERF/      000000
COMMON /CCC/ GRAPH,JOUT,DEMAND      000000
COMMON /CCC/ GRAPH,JOUT,DEMAND      000000
DATA ICASE/O/      000000
DOUBLE PRECISION ASQ,USQ      000000
LOGICAL AREA,EQL,FROZ,HP,SEQL,SP,THI,TP      000000
NAMELIST /RATIMP/ EQL,FROZ,IGAM,PCP,SUBAR,SUPAR      /RATIMP/      000000
NFZ = 1      000000
APP(1) = 1.      000000
IF (ICASE -GT- 0) GO TO 303      000001
00120 31*      000003

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00122 32* ICASE = 1
00123 33* IGAM = 0
00124 34* DO 300 I=1,26
00127 35* PCP(I) = 0.
00130 36* SUBAR(I) = 0.0
00132 37* EQL = .TRUE.
00133 38* F02 = .FALSE.
00134 39* WRITE (6,302)
00136 40* FORMAT (' BEGIN NAMELIST RKTINP INPUT')
00137 41* 302
00142 42* 303 READ (5,RKTINP)
00143 43* NPP = 0
00146 44* DO 305 I = 1,26
00150 45* IF (PCP(I) .LE. 0.0) GO TO 306
00152 46* 305 NPP = I
00153 47* 306 NPP = NPP+2
00154 48* NSUB = 0
00155 49* NSUP = 0
00160 50* DO 320 J=1,13
00162 51* IF (SUBAR(I) .GT. 0.0) NSUB = NSUB + 1
00165 52* IF (SUPAR(I) .GT. 0.0) NSUP = NSUP + 1
00170 53* WRITE (JOUT,RKTINP)
00171 54* SEQL = EQL
00172 55* IOF = 0
00173 56* II = 3800.
00174 57* C LOOP FOR EACH O/F
00175 58* 321 IT = 1
00176 59* IOF = IOF + 1
00177 60* OF = OF(IOF)
00201 62* CALL NEWOF
00201 63* IF (IT) .LE. 0.0) GO TO 322
00202 64* IT = IT+1
00205 65* C LOOP FOR CHAMBER PRESSURES
00206 66* 322 DO 998 IP = 1,MP
00207 67* ITNUM = 0
00211 68* AREA = .FALSE.
00213 69* IF (IT) .LE. 0.0) HP = .TRUE.
00214 70* SP = .FALSE.
00215 71* EQL = .TRUE.
00216 72* ISUB = 1
00217 73* ISUP = 1
00220 74* PP = P(IP)
00220 75* IPP = 1
00221 76* C LOOP FOR PRESSURE RATIOS
00222 77* 331 IF(EQL) GO TO 3.2
00223 78* CALL FROZEN
00225 79* GO TO 1332
00225 80* 332 CALL EQLBRM
00226 81* C
00230 82* 333 IF (IPP.GT.1) GO TO 195
00232 83* 1332 IF (IT .GT. 0.0) GO TO 333
00233 84* IF INPT .LT. 2) RETURN
00233 85* GO TO 900
00235 86* C COMBUSTION CHAMBER
00236 87* EQL = SEQL
TP = .FALSE.

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ROCK0060
ROCK0062

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00237 080 MP = .FALSE.
00239 090 SP = .TRUE.
00241 900 SO = SSUM(I1)
00242 910 CPRF = CP SUM
00243 920 334 TMELT=0.
00244 930
00245 940
00246 950
00247 960
00248 970
00249 980
00250 990
00251 1000
00252 1010
00253 1020
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00265 1140
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01010 8590
01011 8600
01012 8610
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01020 8690
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01050 8990
01051 9000
01052 9010
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01061 9100
01062 9110
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01071 9200
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01081 9300
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01149 9980
01150 9990
01151 10000
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01333 11820
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00354 149*      APPL = PCPLT/(SUBAR(ISOB)*(10.507*ELM**2.9+.454)*ELM)
00355 150*      IF (ARATIO.LT.1.00) APPL = .9*APPL
00357 160*      GO TO 859
00360 170*      799 IF (SUPAR(ISOUP).LT.2.) GO TO 805
00362 180*      IF (ISUP.GT.1.AND.SUPAR(ISOUP-1).GE.2.) GO TO 802
00364 190*      APPL = GAMMA3(2)*ELM*.1.8
00365 150*      GO TO 859
00366 151*      805 APPL = SORT(ELM*(11.535+3.294*ELM)) + PCPLT
00367 152*      GO TO 859
00370 153*      810 IF (IDEBUE .LE. 0 OR NPT .LT. IDEBUG) GO TO 809
00372 155*      WRITE(JOUT,181) ITNUM,ARATIO,AEAT(NPT),APP(NPT),DLMP
00401 155*      1811 FORMAT(18HITER=12,5X,15HASSIGNED AEAT=,F15.8,5X,8HAE/AT=,F15.8,
00401 156*      15X,5HPC/P=,F15.6,5X,13HDELTA LN P=,F15.8)
00402 157*      809 TOL = 1.0E-5
00403 158*      IF (ARATIO .GE. 10.0) TOL = .40E-5
00405 159*      IF (ABS(AEAT(NPT)) - ARATIO)/ARATIO .LT. TOL GO TO 830
00407 160*      IF (ABS(DLMP) .LT. .40E-6) GO TO 830
00411 161*      AEATL = ALG(AEAT(NPT))
00412 162*      ITNUM = ITNUM + 1
00413 163*      IF (ITNUM .GT. 25) GO TO 820
00415 164*      ASO = RBR*GAMMA5(NPT)*ENN*TT
00416 165*      DLMP = GAMMA5(NPT)*USO/(USO-ASO)
00417 166*      802 DLMP = DLMP*ELM-DLMP*AEATL
00420 167*      APPL = APPL + DLMP
00421 168*      IF (ITNUM.EQ.1) GO TO 859
00423 169*      APP(NPT) = EXP(1*APPL)
00424 170*      PP = P(IP1)/APP(NPT)
00425 171*      GO TO 331
00426 172*      820 WRITE(JOUT,821) ARATIO
00431 173*      821 FORMAT(12HROCKET DID NOT CONVERGE FOR AREA_RATIO =,F11.6/)
00432 174*      830 ITNUM = 0
00433 175*      AEAT(NPT) = ARATIO
00434 176*      IF (MSUB.LE.0) GO TO 834
00436 177*      ISUB = ISUB + 1
00437 178*      IF (ISUB .LE. NSUB) GO TO 800
00441 179*      2SUB = 1
00442 180*      NSUB = -NSUB
00443 181*      IF (ISUP.LE.NSUP) GO TO 800
00445 182*      GO TO 835
00446 183*      834 ISUP = ISUP + 1
00447 184*      IF (ISUP.LE.NSUP) GO TO 800
00451 185*      ISUP = 1
00452 186*      835 AREA = .FALSE.
00453 187*      GO TO 860
00454 188*      859 ISV = NPT
00455 189*      IF (NPT.NE.13) GO TO 870
00457 190*      860 CALL RKTOUT (IGAM)
00460 191*      IF (TT .LE. 0.0) ISV = 0
00462 192*      IF (.NOT. EQL .AND. TT .LE. 0.0) WRITE(JOUT,862)
00465 193*      862 FORMAT(12H,125H-CALCULATIONS WERE STOPPED IN ROCKET BECAUSE NEXT
00465 194*      2ED SPECIES)
00466 195*      IF (ISV.EQ.0) GO TO 900
00470 197*      IDEBUG = IDEBUG-13
00471 198*      WRITE(JOUT,865)
00473 199*      865 FORMAT(11H)

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ROCK00080

ROCKET

DATE 101500

PAGE

6

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00474 200*      NPT = 2
00475 201*      870 IF (.NOT.EQL) GO TO 880
00476 202*      IF (ISV.EQ.1) ISV = -1
00500 203*      CALL SAVE
00502 204*      880 IPP = IPP+1
00503 205*      IF (NPT.EQ.2) GO TO 331
00504 206*      IF (.NOT.AREA) APP(NPT)=PCPIPP-2)
00506 207*      IF (AREA) APP(NPT)=EXP(APPL)
00510 208*      PP = P(IPP)/APP(NPT)
00512 209*      GO TO 331
00513 210*      990 IF (LOGUE.LT.0) IDEBUG=IDEBUG+13
00514 211*      IF (NSUB.LT.0) NSUB=-NSUB
00516 212*      IF (.NOT.FROZ.OR..NOT.EQL) GO TO 997
00520 213*      CPR(1) = CPRF
00522 214*      GAMMA(1) = CPRF/(CPRF-1./WM(1))
00523 215*      YT = YTT(1)
00524 216*      IPP = 1
00525 217*      NPT = 1
00526 218*      CALL SAVE
00527 219*      EQL = .FALSE.
00530 220*      ENN = 1./WM(1)
00531 221*      GO TO 334
00532 222*      997 NPT = 1
00533 223*      WRITE(JOUT,865)
00534 224*      IF (EQL) CALL SAVE
00536 225*      998 IT = TTT(1)
00540 226*      IF (IT.GE.NT) GO TO 999
00542 227*      IT = IT+1
00544 228*      TT = TTT(1)
00545 229*      GO TO 322
00546 230*      999 IF (IOF.GE.NOF) RETURN
00547 231*      GO TO 321
00551 232*      END
00552 233*      END
```

ROCK0121

ROCK0129

END OF COMPILATION: NO DIAGNOSTICS.

AMG,P READ

FOR S READ READ
MSA 'E3 -10/15/80-13:07:40 (26,)

SUBROUTINE READ ENTRY POINT 001330

STORAGE USED: CODE(1) 001345; DATA(10) 001373; BLANK COMMON(2) 000000

COMMON BLOCKS:

0003 CFUEL 000001

EXTERNAL REFERENCES (BLOCK, NAME)

0004 ROYES
0005 PAGII
0006 CHRISZ
0007 GOUT
0010 MNCODS
0011 RDATAI
0012 RDATAF
0013 DMRTF
0014 ROCHAR
0015 MREWS
0016 MRBUS
0017 MI02S
0020 MI01S
0021 MERR2S
0022 MRBUS
0023 MVEFS
0024 MERR3S

STORAGE ASSIGNMENT (BLOCK, TYPE, RELATIVE LOCATION, NAME)

0001	000014	10L	0001	000277	100L	0001	000375	106L	0001	000437	110L	0001	000517	120L
0001	000551	130L	0001	000605	140L	0001	000623	150L	0001	000644	160L	0001	000662	170L
0001	000041	176G	0001	000703	200L	0001	00045	2026	0001	000116	2326	0001	000134	2426
0001	000747	300L	0001	001032	310L	0001	000326	3226	0001	001062	330L	0001	001110	340L
0001	000366	344G	0001	001127	350L	0001	001144	360L	0001	000454	3656	0001	001161	370L
0001	000501	376G	0001	001201	400L	0001	001216	408L	0001	001305	420L	0001	000716	4506
0001	000717	453G	0001	000070	50L	0001	000770	5016	0001	001015	5126	0001	001210	5656
0001	001231	602G	0001	001235	606G	0001	001276	635G	0001	000177	70L	0000	001276	802F
0001	000240	90L	0001	000274	95L	0000	R 000226	ANUM	0003	R 000000	CF	0000	R 000702	DENS
0000	R 000536	ENTH	0000	R 001125	EXMPIA	0000	R 001140	EXMPIR	0000	R 001150	EXMP2	0000	R 001156	EXMP2B
0000	R 001163	EXMP3	0000	R 001170	EXMP3B	0000	R 001177	EXMP4	0000	R 001203	EXMP5	0000	R 001207	EXMP6
0000	R 001214	EXMP7	0000	R 000567	FAZ	0000	R 000651	FOX	0000	I 001252	I	0000	I 001257	ICHNG
0000	001347	INJPS	0000	I 001250	IO	0000	I 001255	IOPT	0000	I 001023	ICUT	0000	I 001220	IRZACT
0000	I 001253	J	0000	I 001256	LINEO	0000	I 000733	LINE1	0000	I 000760	LINE2	0000	I 001003	LINE3
0000	I 001050	MODIFY	0000	I 001065	MODMEN	0000	I 000535	MOLE	0000	I 001256	N	0000	I 000000	NAME
0000	I 001254	MAST	0000	I 001260	NDUHTY	0000	I 001251	NREAC	0000	I 001246	N3	0000	I 001247	N8
0000	R 000454	PECUT	0000	R 001224	RDUM	0004	L 000000	ROYES	0000	R 000620	RTEMP			

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00101 10 SUBROUTINE RREAD(FIRST) 000000
00102 20 LOGICAL FIRST,RYES 000000
00103 30 C 000000
00103 40 C 000000
00103 50 C 000000
00103 60 C 000000
00104 70 C 000000
00104 80 C 000000
00104 90 C 000000
00104 100 C 000000
00104 110 C 000000
00104 120 C 000000
00104 130 C 000000
00104 140 C 000000
00104 150 C 000000
00104 160 C 000000
00104 170 C 000000
00104 180 C 000000
00104 190 C 000000
00104 200 C 000000
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00104 490 C 000000
00104 500 C 000000
00104 510 C 000000
00104 520 C 000000
00104 530 C 000000
00104 540 C 000000
00104 550 C 000000

SUBROUTINE RREAD(FIRST)
LOGICAL FIRST,RYES

USE MIPS INPUT ROUTINES TO READ REACTANT CARDS (STORE ON FILE 8)

DATA ARRAYS FOR REACTANT CARDS
DIMENSION NAME(25,6),ANUM(25,6),PECNT(25),MOLE(25),ENTH(25),
X FAZ(25),RTEMP(25),FOX(25),DENS(25)

COMMON /CFUEL/CF
ARRAYS FOR DATA MENU'S
DIMENSION LINE(21),LINE2(19),LINE3(16),IOUT(21),MODIFY(13)
DIMENSION MODMEN(4,8),EXMP1A(11),EXMP1B(8),EXMP2(6),EXMP2B(5),
EXMP3(5),EXMP3B(7),EXMP4(9),EXMP5(4),EXMP6(5),EXMP7(4),
IReact(4),ROUM(10),LINED(8)

SET DATA ARRAYS FOR MENU'S
DATA LINED,6MTYPE,6HYES 1,6MO REA,6M IN PR,6MEVIOUS,
1 6M REACT,6MANT SE,6MT / 6MREACTA,6MNT(4),3*6M
DATA LINE3,6M INDEX,4,6M / 6MREACTA,6MNT(4),3*6M
1 6M R,6MEL WT/,6M MOL,6ME,ENT,6MHALPY/,6M PHA,6MSE TE,
2 6MMP,N,6M FUEL/,6M DENS,6MHITY / 6M N,6MO,MOLE,6MWS,6M INT.
DATA LINE2,10,6M / 6M N,6MO,MOLE,6MWS,6M INT.
1 6M ENRG,6M / 6M OXID / 6M IND,6MHCATES,6M ENTHA.
DATA LINE3,8,6M / 6M N,6MO,MOLE,6MWS,6M INT.
1 6MPLY TO,6M BE CA,6MCLCAT,6MED / 6M IND,6MHCATES,6M ENTHA.
DATA MODMEN,24M 1-REACTANT FORMULA / 6M IND,6MHCATES,6M ENTHA.
1 24M 2-REL WT/NO MOLES / 6M IND,6MHCATES,6M ENTHA.
2 24M 3-PHASE (S-L-G) / 6M IND,6MHCATES,6M ENTHA.
3 24M 6-FUEL,OXIDIZER (F/O) / 6M IND,6MHCATES,6M ENTHA.
4 24M RETURN TO CONTINUE / 6M IND,6MHCATES,6M ENTHA.
1 304, MOLLERINTM CODE FOR SYMBOLS / 6M IND,6MHCATES,6M ENTHA.
DATA EXMP1A,36M TYPE CHEMICAL FORMULA THIS REACTANT,
DATA EXMP1B,48M EXAMPLE CARBON TETRACHLORIDE IMC 1. 2MCL 4. /
DATA EXMP2,36M TYPE REL WEIGHT/NUMBER OF MOLES / 6M IND,6MHCATES,6M ENTHA.
DATA EXMP2B,30M TYPE YES IF VALUE IS MOLES / 6M IND,6MHCATES,6M ENTHA.
DATA EXMP3,30M TYPE ENTHALPY/INTERNAL ENERGY / 6M IND,6MHCATES,6M ENTHA.
DATA EXMP3B,24M TYPE YES IF ENTHALPY TO BE CALCULATED / 6M IND,6MHCATES,6M ENTHA.
DATA EXMP4,24M TYPE PHASE (S-L-G) / 6M IND,6MHCATES,6M ENTHA.
DATA EXMP5,24M TYPE TEMPERATURE (K) / 6M IND,6MHCATES,6M ENTHA.
DATA EXMP6,30M TYPE FUEL/OXIDIZER (F/O) / 6M IND,6MHCATES,6M ENTHA.
DATA EXMP7,24M TYPE DENSITY (G/CC) / 6M IND,6MHCATES,6M ENTHA.
DATA MODIFY,6M TYPE,6M 1, 2,6MOR 3,6MTO MOD,6MHIFY, D,
1 6MELETE,6M OR AD,6MD A RE,6MACTANT,6M (RETO,6MRN TO,
2 6MCONTIN,6MUE) / 6M IND,6MHCATES,6M ENTHA.
DATA IReact,24M TYPE REACTANT NUMBER / 6M IND,6MHCATES,6M ENTHA.
DATA N3,8/,NB,12/

CALL PAGIT
IO=N3
NREAC=0
FOR FIRST PASS DO NOT CHECK SAVED DATA
IF (.NOT. FIRST) GO TO 10
IF (.NOT. RYES (LINED,43)) GO TO 50

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00162 56* C
00162 57* C
00164 58* 10
00165 59*
00167 60*
00173 61*
00175 62*
00200 63*
00200 64*
00220 65*
00220 66*
00220 67*
00220 68*
00222 69*
00223 70*
00224 71*
00225 72*
00227 73*
00230 74*
00231 75*
00234 76*
00235 77*
00237 78*
00237 79*
00257 80*
00260 81*
00262 82*
00263 83*
00264 84*
00265 85*
00266 86*
00267 87*
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00276 93*
00277 94*
00300 95*
00302 96*
00303 97*
00304 98*
00305 99*
00307 100*
00310 101*
00310 102*
00310 103*
00312 104*
00313 105*
00314 106*
00315 107*
00317 108*
00317 109*
00337 110*
00340 111*

      READ IN PRESENT CASE
      CONTINUE
      IF (ITO.EQ.N3) REMIND IO
      READ (IO) NREAC,CF
      IF (NREAC.LT.1) GO TO 50
      DO 25 I=1,NREAC
      READ (IO) (NAME(I,J),ANUM(I,J),J=1,5),PECUT(I),MOLE(I),
      ENTH(I),NAME(I,6),ANUM(I,6),FAZ(I),RTEMP(I),FOX(I),DENS(I)
      CONTINUE
      X
      25
      C
      DISPLAY PRESENT SET OF REACTANTS (ADD IF NONE EXISTS)
      CONTINUE
      CALL PAGIT
      CALL CHRSTZ(4)
      IF (NREAC.LT.1) GO TO 70
      CALL GOUTLINE1,125)
      CALL GOUTLINE2,119)
      DO 60 I=1,NREAC
      NAST=1H
      IF (NAME(I,6).EQ.2H00) NAST=1H
      ENCODE(02,1OUT),1,(NAME(I,J),ANUM(I,J),J=1,5),PECUT(I),MOLE(I),
      X ENTH(I),NAST,FAZ(I),RTEMP(I),FOX(I),DENS(I),
      CALL GOUTLINE1,125)
      CONTINUE
      60
      C
      CALL GOUT(' ',1)
      CALL GOUTLINE3,92)
      CALL GOUT(' ',1)
      CONTINUE
      70
      C
      CALL GOUT(MODIFY,75)
      IOPT=0
      CALL RDATA(1,IOPT,870)
      IF (IOPT.LT.0 .OR. IOPT.GT.3) GO TO 70
      IF (IOPT.EQ.0) GO TO 400
      GO TO (90,90,300),IOPT
      C
      C
      SELECT REACTANT NUMBER
      CONTINUE
      N=1
      IF (NREAC.EQ.1) GO TO 95
      N=0
      CALL GOUT(IREACT,24)
      CALL RDATA(1,N,990)
      IF (N.LT.1 .OR. N.GT.NREAC) GO TO 90
      CONTINUE
      95
      IF (IOPT.EQ.2) GO TO 200
      C
      C
      SELECT MODIFICATION OPTIONS
      CONTINUE
      CALL PAGIT
      NAST=1H
      IF (NAME(I,6).EQ.2H00) NAST=1H
      ENCODE(02,1OUT),1,(NAME(I,J),ANUM(I,J),J=1,5),PECUT(I),MOLE(I),
      X ENTH(I),NAST,FAZ(I),RTEMP(I),FOX(I),DENS(I),
      CALL GOUTLINE1,125)
      CALL GOUTLINE2,114)
      111*

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READ

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00391 1120 CALL GOUT(IOUT,125) 000353
00392 1130 CALL GOUT(I,1) 000387
00393 1140 DO 105 I=1,6 000346
00394 1150 CALL GOUT(MODMEM(1,1),29) 000346
00397 1160 105 CONTINUE 000375
00398 1170 106 CONTINUE 000375
00399 1180 ICHNG=0 000375
00400 1190 CALL RDATA(I1,ICMNG,S106) 000375
00401 1200 IF (ICMNG.EQ.0) GO TO 50 000402
00402 1210 IF (ICMNG.LT.1 .OR. ICMNG.GT.7) GO TO 104 000404
00403 1220 GO TO (110,120,130,140,150,160,170),ICMNG 000422
00404 1230 110 CONTINUE 000437
00405 1240 CALL GOUT(EMP1A,66) 000437
00406 1250 CALL GOUT(EMP1B,98) 000442
00407 1260 DO 112 I=1,5 000454
00408 1270 J=(I-1)*2 + 1 000454
00409 1280 RDMU(I)=2H 000461
00410 1290 RDMU(J)=120 000464
00411 1300 112 CONTINUE 000467
00412 1310 CALL RDATA(I10,RDMU,S110) 000467
00413 1320 DO 114 I=1,5 000501
00414 1330 J=(I-1)*2 + 1 000501
00415 1340 FLD(0,36,NAME(N,I))=FLD(0,36,RDMU(J)) 000507
00416 1350 C CALL CHECKNAME(N,I) 000507
00417 1360 ANUMIN,I=RDMU(J+1) 000511
00418 1370 CONTINUE 000511
00419 1380 GO TO 100 000515
00420 1390 C 000515
00421 1400 120 CONTINUE 000517
00422 1410 CALL DMWRT(EMP2,36,PECMIN),S) 000527
00423 1420 CALL RDATA(I1,PECMIN),S120) 000536
00424 1430 MOLEIN)=3H 000540
00425 1440 IF (.NOT.ROYES(EMP2B,30)) GO TO 100 000548
00426 1450 MOLEIN)=3H 000547
00427 1460 GO TO 100 000547
00428 1470 C 000551
00429 1480 130 CONTINUE 000551
00430 1490 CALL DMWRT(EMP3,30,ENTH(N),S) 000551
00431 1500 CALL RDATA(I1,ENTH(N),S130) 000561
00432 1510 NAMEIN,6)=2H 000570
00433 1520 IF (ROYES(EMP3B,92)) NAME(N,6)=2H00 000573
00434 1530 GO TO 100 000603
00435 1540 C 000603
00436 1550 140 CONTINUE 000605
00437 1560 CALL GOUT(EMP4,29) 000611
00438 1570 CALL ROCHAR(FAZ(N),1,1,S140) 000621
00439 1580 GO TO 100 000621
00440 1590 C 000621
00441 1600 150 CONTINUE 000623
00442 1610 CALL DMWRT(EMP5,29,RTMPIN),S150) 000623
00443 1620 CALL RDATA(I1,RTMPIN),S150) 000633
00444 1630 GO TO 100 000642
00445 1640 C 000642
00446 1650 160 CONTINUE 000644
00447 1660 CALL GOUT(EMP6,30) 000644
00448 1670 CALL ROCHAR(FOX(N),1,1,S160) 000650
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00440 1690 60 TO 100
00440 1690 C
00441 1700 CONTINUE
00442 1710 CALL DMRTF(EMP7,24,DENS(N),S)
00443 1720 CALL RDATAF1,DENS(N),S170)
00444 1730 GO TO 100
00444 1740 C
00444 1750 C
00445 1760 200
00446 1770 CONTINUE
00447 1780 NREAC=NREAC-1
00448 1790 DO 220 I=N,NREAC
00449 1800 NAME(I,J)=NAME(I+1,J)
00450 1810 AMUM(I,J)=AMUM(I+1,J)
00451 1820 CONTINUE
00452 1830 PECHT(I)=PECHT(I+1)
00453 1840 MOLE(I)=MOLE(I+1)
00454 1850 ENTH(I)=ENTH(I+1)
00455 1860 FAZ(I)=FAZ(I+1)
00456 1870 RTEMP(I)=RTEMP(I+1)
00457 1880 FOX(I)=FOX(I+1)
00458 1890 DENS(I)=DENS(I+1)
00459 1900 CONTINUE
00460 1910 60 TO 50
00461 1920 C
00462 1930 C
00463 1940 300
00464 1950 NREAC=NREAC-1
00465 1960 N=NREAC
00466 1970 CALL GOUT(EMPJA,66)
00467 1980 CALL GOUT(EMP18,66)
00468 1990 DO 305 I=1,6
00469 2000 J=(I-1)*2 + 1
00470 2010 RDM(J)=2H
00471 2020 RDM(J+1)=0.
00472 2030 CONTINUE
00473 2040 CALL RDATAF10,RDM,S300)
00474 2050 DO 307 I=1,5
00475 2060 J=(I-1)*2 + 1
00476 2070 FLDIO,36,NAME(N,I)=FLDIO,36,RDM(J)
00477 2080 CALL CHECKNAME(N,I)
00478 2090 AMUM(N,I)=RDM(J+1)
00479 2100 CONTINUE
00480 2110 307
00481 2120 310
00482 2130 CONTINUE
00483 2140 CALL GOUT(EMP2,36)
00484 2150 PECHT(N)=0.
00485 2160 CALL RDATAF1,PECHT(N),S310)
00486 2170 CONTINUE
00487 2180 MOLE(N)=1H
00488 2190 IF (GYES(EMP28,30)) MOLE(N)=1H
00489 2200 CONTINUE
00490 2210 CALL GOUT(EMP3,50)
00491 2220 ENTH(N)=0.
00492 2230 CALL RDATAF1,ENTH(N),S330)
00493 2240 IF (GYES(EMP38,42)) NAME(N,6)=2H00
00494 2250 CONTINUE
00495 2260 340
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READ

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00500 2200 CALL GOUTIEXP(29)
00501 2250 FAZIN)=1WS
00502 2260 CALL RDCMAR(FAZIN),1,-1,0340)
00503 2270 CONTINUE
00504 2280 CALL GOUTIEXP(29)
00505 2290 RTEMPIN)=0.
00506 2300 CALL RDATAF(1,RTEMPIN),0350)
00507 2310 CONTINUE
00508 2320 CALL GOUTIEXP(30)
00509 2330 FOXIN)=1WF
00510 2340 CALL RDCMAR(FOXIN),1,-1,0360)
00511 2350 CONTINUE
00512 2360 CALL GOUTIEXP(29)
00513 2370 DENSIN)=0.
00514 2380 CALL RDATAF(1,DENSIN),0370)
00515 2390 GO TO 50
00516 2400 C
00517 2410 C
00518 2420 STORE CASE TO FILE A
00519 2430 CONTINUE
00520 2440 REMIND IO
00521 2450 IF (IO-NO) 60 TO 900
00522 2460 DO 906 I=1,5
00523 2470 READ (IO) MUMMY
00524 2480 CONTINUE
00525 2490 CONTINUE
00526 2500 WRITE (IO) NREAC,CF
00527 2510 DO 910 I=1,NREAC
00528 2520 WRITE (IO) (NAME(I),J),ANUM(I,J),J=1,5),PECUT(I),MOLE(I),
00529 2530 ENTHT(I),NAME(I,6),ANUM(I,6),FAZIN),RTEMP(I),FOXIN),DENS(I)
00530 2540 X
00531 2550 CONTINUE
00532 2560 IF (IO-NO) 60 TO 920
00533 2570 IF (I-NOT,ROYESI) TYPE YES TO EDIT COAL REACTANT DATA',35))
00534 2580 X
00535 2590 GO TO 920
00536 2600 IO=NO
00537 2610 REMIND IO
00538 2620 DO 912 I=1,5
00539 2630 READ (IO) MUMMY
00540 2640 CONTINUE
00541 2650 912 GO TO 10
00542 2660 920 ENDFILE IO
00543 2670 RETURN
00544 2680 002 FORMAT(1X,12,2X,5,12,70,9,2X),F10.6,2X,A1,F13.6,A1,3X,A1,F12.3,
00545 2690 1 3X,A1,F12.5,1X)
00546 2700 END
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8 FOR S SAVE SAVE
MSA E3 -10/15/80-13:07:45 (13.1)

SUBROUTINE SAVE ENTRY POINT 000501
MEMOR ENTRY POINT 000504

STORAGE USED: CODE(1) 000507; DATA(0) 000104; BLANK COMMON(2) 000000

COMMON BLOCKS:

0003 COMSTS 000004
0004 MOLCOM 000010
0005 SPECS 017106
0006 MISC 001701
0007 INDX 000041
0010 ECC 000001
0011 CFUEL 000004

EXTERNAL REFERENCES (BLOCK, NAME)

0012 MCALC
0013 EXP
0014 MWDUS
0015 MIOZS
0016 MIOIS
0017 MERRIS

STORAGE ASSIGNMENT (BLOCK, TYPE, RELATIVE LOCATION, NAME)

0001	000137	100L	0001	000056	13L	0001	000042	1326	0001	000073	15L	0001	000112	20L	
0001	000172	200L	0001	000161	201G	0001	000207	2106	0001	000326	2526	0001	000291	302L	
0001	000435	317G	0001	000127	50L	0000	000014	730F	0000	000017	732F	0001	000313	744L	
0001	000322	745L	0001	000356	750L	0001	000365	760L	0000	000035	770F	0000	000045	780F	
0000	000050	785F	0005	011052	A	0006	000640	AM	0006	000705	AM1	0006	001135	ANUP	
0003	000000	ATM4	0006	000004	ATOM	0006	000514	BO	0006	000545	JNP	0007	000036	CALCH	
0011	R	000000	0005	000000	COEF	0000	000006	COF	0007	000001	CONVE	0006	000706	CPRI	
0006	000634	CPSLIN	0006	000654	DATA	0005	010624	DELM	0010	000002	DEMAND	0006	001560	DEMS	
0005	R	000312	0004	000000	END	0005	R	010150	0006	R	001700	0006	000000	ENM	
0006	R	001674	0006	R	001677	0000	001414	ENTH	0006	R	000636	0006	001445	F42	
0000	R	000003	0000	R	000013	FF	0000	000002	0006	R	001527	0000	000001	FUU	
0004	000001	G4S	0003	000001	GMET	0000	000000	GRAPH	0011	000001	HMV	0007	000003	MP	
0006	R	000642	0000	R	000012	MS	0006	P	0000	010376	MO	0007	000030	IC	
0007	000000	IOERUG	0004	I	000002	IE	0007	000015	0000	000057	INJPS	0007	000023	IOMS	
0007	000021	IP	0007	I	000037	IQSAVE	0007	I	000016	IO1	000005	ISV	0007	000034	IT
0005	I	001626	0004	000003	IZERO	0000	000005	J	0007	I	000026	JLIQ	0010	000001	JOUT
0007	I	000025	0007	C	00031	J51	0007	000014	0004	I	000004	LANR	0006	000463	LLMT
0000	I	000004	0007	I	000040	LSAVE	0004	000005	0007	000006	MOLES	0006	000767	MAHF	
0007	000024	MC	0007	000022	MEWR	0007	000035	MFZ	0007	I	000012	MLM	0007	000017	MCF
0007	000020	MCMTT	0007	000007	MP	0007	I	000011	0007	000027	MREAC	0007	I	000013	MS
0000	I	000000	0007	000010	MT	0006	R	000635	0004	000006	OX	0006	001444	OXZ	
0003	000002	PATH	0006	C	00163	PFCHT	0011	R	000003	0006	000633	PP	0003	000003	RBAP
0003	000004	RHR	0006	R	000644	RH	0006	P	001611	0006	001612	RHW	0006	001476	RTEMP

SAVE

DATE 101500

PAGE 2

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00003 RVR 0005 00000 S 0007 00000 SP
015364 SUB 0000 000007 SUM 0006 01660 SM
0006 000632 TMIGM 0006 001643 TLM 0006 000630 TLOW 0006 000627 TM 0006 000631 TMID
0007 000002 TP 0006 000002 TT 0006 000646 VMIM 0007 000032 VOL 0006 000630 VPLS
0000 R 000011 V1 0000 000010 V2 0011 R 000002 MCR 0006 000652 WP 0006 000657 ZERO
  
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00101 10 SUBROUTINE SAVE 000000
00101 20 C 000000
00101 30 C SAYS OR USES COMPOSITIONS FROM PREVIOUS POINT AS INITIAL ESTIMATES 000000
00101 40 C 000000
00101 50 COMMON /CONSTS/ ATMM GNET, PATH, MBAR, RBR, RVR 000000
00101 60 COMMON /MOLCOM/ EM, GAS, IE, IZERO, LAMK, MOL, OX, ZERO 000000
00101 70 COMMON /SPECES/ CREF(12,7,150), S(150), EM(150,13), ENLM(150), MO(150) 000000
00101 80 C 1 DELM(150), (15,150), SUB(150,3), IUSE(150), TEMPI(50,2), SLN(150) 000000
00101 90 INCLUDE SPECES 000000
00101 100 COMMON /MISC/ ENH, SUM, TT, SO, TON(13,101), LLMT(25), BO(25), 000000
00101 110 1 BOPI(25,2), TM, TLOW, TMID, THIGH, PP, CP, SUM, OPE, ORAT, 000000
00101 120 2 MSUBO, AM(2), MPP(2), AM(2), VMIM(2), VPLS(2), MP(2), 000000
00101 130 3 DATA(25), AM1, CPRI, NAME(25,6), ANUM(25,6), PECNT(25), 000000
00101 140 4 EM(125), FAZ(25), RTEMP(25), FOX(25), DENSI(25), RMOP, 000000
00101 150 5 RMV(25), TLM, OXE(26), ENML, EMSAVE, EALSAV 000000
00101 160 COMMON /INDX/ IODEBUG, COMVG, TP, MP, SP, ISV, MOLES, MP, NT, MPT, M, M, NS, 000000
00101 170 1 KMAT, IMAT, IOL, MOP, MONIT, IP, MEWR, IONS, MC, JSOL, JLIQ, 000000
00101 180 2 MREAC, IC, JSI, VOL, SHOCK, IT, MFZ, CALCH, IOSAVE, LSAVE 000000
00101 190 3 000000
00101 200 COMMON /CCC/ GRAPH, JOUT, DEMAND 000000
00101 210 COMMON /CFUEL/ CF, MHV, MCH, PER 000000
00101 220 000000
00101 230 DATA FUU/AMU, C/FMW/AMM, C/FCL/AMAL/B/ 000000
00101 240 LOGICAL CALCH, IONS, VOL 000000
00101 250 000000
00101 260 C IF(ISOV100,10,200) 000000
00101 270 C NEXT POINT FIRST IN SCHEDULE, USE PREVIOUS COMPOSITIONS FOR THIS 000000
00101 280 10 IOL = IOSAVE 000000
00101 290 ENH = EMSAVE 000000
00101 300 ENML = EMLSAV 000000
00101 310 LLI = MLM 000000
00101 320 DO 50 J = 1, NS 000000
00101 330 IF (I, MOT, IONS, OR, LLMT(MLM), CO, LSAVE, 60 TO 15 000000
00101 340 IF (LL, T(LML), CO, IE: 60 TO 13 000000
00101 350 IF (IUSE(J), ME, -10000) 60 TO 15 000000
00101 360 IUSE(J) = 0 000000
00101 370 LLI = MLM+1 000000
00101 380 GO TO 20 000000
00101 390 13 IF (SLM(J), ME, 0, OR, IUSE(J), ME, 0) 60 TO 15 000000
00101 400 LLI = MLM+1 000000
00101 410 IUSE(J) = -10000 000000
00101 420 GO TO 50 000000
00101 430 15 IF (IUSE(J), FO, 0) 60 TO 20 000000
00101 440 EN (J, MPT) = SLM(J) 000000
00101 450 IF (IUSE(J), GT, 0) IUSE(J) = - IUSE(J) 000000
00101 460 IF (EN(J, MPT), GT, 0, 0) IUSE(J) = - IUSE(J) 000000
00101 470 GO TO 30 000000
  
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00162 48* 20 EN(J,NPT) = 0.
00163 49* EN(J) = SLN(J)
00164 50* IF (ENLN(J) + 10.50 .LE. ENNL) GO TO 50
00166 51* EN(J,NPT) = EXP(ENLN(J))
00167 52* 50 CONTINUE
00171 53* NLN = LL1
00172 54* RETURN
00173 55* C FIRST T-SAVE COMPOSITIONS FOR FUTURE POINTS WITH THIS T
00174 56* 100 ISV = -ISV
00175 57* IQSAVE = IQ1
00176 58* FMSAVE = FMM
00177 59* FMSAV = ENNL
00178 60* LSAVE = LLMT(NLM)
00179 61* DO 150 J = 1,NS
00180 62* SLN(J) = ENLN(J)
00181 63* 150 IF (IUSE(J) .NE. 0) SLN(J) = EN(J,ISV)
00182 64* C USE COMPOSITIONS FROM PREVIOUS POINT
00183 65* 200 DO 300 J = 1,NS
00184 66* 300 EN(J,NPT) = EN(J,ISV)
00185 67* RETURN
00186 68* C CALCULATE NEW VALUES OF 80 AND HSUBD FOR NEW OF RATIO
00187 69* ENTRY NEWOF
00188 70* WRITE(JOUT,730) OF
00189 71* 730 FORMAT(6HOF = ,F10.6)
00190 72* IF (CF+1.0) ,302,
00191 73* COF=OF/CF
00192 74* WRITE (JOUT,732) COF,WCR,PER
00193 75* 732 FORMAT (21X,'OXIDIZER/COAL=',F8.4,5X,'WATER/COAL=',F8.4,
00194 76* 5X,'CARBON CONVERSION=',F8.4)
00195 77* 302 CONTINUE
00196 78* SUM = OF + 1.
00197 79* V2 = (OF+VMIN(1)+VMIN(2))/SUM
00198 80* V1 = (OF+VPLS(1)+VPLS(2))/SUM
00199 81* IF (V2 .LT. 0.0) EGRAT = ABS(V1/V2)
00200 82* IF (RH(1) .GT. 0.0 .AND. RH(2) .GT. 0.0) GO TO 744
00201 83* RHOP = RH(2)
00202 84* IF (RHOP .LE. 0.0) RHOP = RH(1)
00203 85* GO TO 745
00204 86* 744 RHOP = (OF+1.)*RH(1)+RH(2)/(RH(1)+ OF *RH(2))
00205 87* 745 DO 747 J = 1,NLM
00206 88* 747 B(J) = (ROP(J,2) + FOP(J,1)*OF)/SUM
00207 89* NPT = 1
00208 90* IF (.NOT.CALCH) GO TO 750
00209 91* CALL HCALC
00210 92* CALCH = .FALSE.
00211 93* IF (OF .GT. 0.0) HPP(1) = SUM*HPP(1)/OF
00212 94* HPP(2) = SUM*HPP(2)
00213 95* GO TO 760
00214 96* 750 HSUBD = (HPP(2) + HPP(1)*OF)/(RBAR*SUM)
00215 97* 760 IC = 0
00216 98* JSOL = 0
00217 99* JULIC = 0
00218 100* HS = PRAR*HSUBD
00219 101* WRITE(JOUT,770)
00220 102* 770 FORMAT (1H0,17X,4HFUEL ,13X,7HOXIDANT ,12X,7HMINATURE //)
00221 103* 780 FORMAT (1H 24X,3E10.8/)

```

SAVE	DATE 101500	PAGE 9
00300	104*	000377
00301	105*	000401
00303	106*	000405
00312	107*	000421
00314	108*	000426
00315	109*	000426
00327	110*	000444
00330	111*	000506

```

FF = FWH
IF (VOL)FF = FWH
WRITE(1,OUT,780) FF,FCAL ,HPP(2),HPP(1),MS
WRITE(1,OUT,785)
785 FORMAT (12H MS-ATOMS/MS)
WRITE(1,OUT,790) (ILLMI(I),LANR,BOPI(I,2),BOPI(I,1),BOPI(I,3)) = 1,MMI)
RETURN
END

```

END OF COMPILATION: NO DIAGNOSTICS.

END,P SEARCH

ORIGINAL PAGE IS
OF POOR QUALITY

FOR S SEARCH SEARCH
HSA E3 -10/19/80-13:07:40 (16.)

SUBROUTINE SEARCH ENTRY POINT 000445

STORAGE USED: CODE(1) 000461; DATA(0) 000121; BLANK COMMON(2) 000000

COMMON BLOCKS:

0003 HOLCOM 000010
0004 SPECES 01716
0005 MISC 001781
0006 INDX 000041
0007 CCC 000003

EXTERNAL REFERENCES (BLOCK, NAME)

0010 MOVABS
0011 HOLDIT
0012 PAGIT
0013 GOUT
0014 NREWS
0015 MRDUS
0016 NI02S
0017 NI01S
0020 NUDUS
0021 NERR3S

STORAGE ASSIGNMENT (BLOCK, TYPE, RELATIVE LOCATION, NAME)

0000	000022	10F	0001	000021	125G	0001	000022	130G	0001	000310	145L	000050	146G	
0001	000102	134G	0001	000031	170L	0001	000128	171G	0001	000326	171L	000055	172F	
0001	000126	173G	0000	000055	176F	0000	000030	20F	0001	000144	204G	000154	207G	
0001	000204	220G	0001	000211	225G	0001	000222	233G	0001	000276	254G	000346	277G	
0001	000376	306G	0000	000020	5F	0001	000042	7L	0001	000167	805L	000171	810L	
0001	000225	820L	0001	000234	825L	0000	000032	871F	0004	R 011052	A	000640	AM	
0005	000705	AM1	0005	001139	ANUM	0005	000004	ATOM	0000	R 000001	B	000514	80	
0005	000545	80P	0006	000036	CALCH	0004	R 000000	COEF	0006	000001	COMVG	000704	CPRI	
0005	000634	CPSUM	0005	000654	DATA	0004	R 004312	DATE	0004	010624	DELM	000002	DEMAND	
0005	001560	OEMS	0004	004312	EM	0003	I 000000	END	0004	010150	ENL	001700	ENLSAV	
0005	000000	ENW	0005	001676	ENNL	0005	001677	ENSAVE	0005	001414	EMTH	000636	EORAT	
0005	001445	FAZ	0005	001527	FOX	0003	I 000001	GAS	0007	000000	GRAPH	000003	HP	
0005	000642	HPP	0005	000637	MSUBO	0004	010376	HO	0000	I 000013	I	000030	IC	
0006	000000	IDEBUG	0003	000002	IE	0006	000015	IMAT	0000	000073	INJPS	000023	IONS	
0006	000021	IP	0006	000037	IOSAVE	0006	000016	IOI	0006	000005	ISV	000034	IT	
0004	I 016266	IUSE	0000	I 000012	IX	0006	000003	IZERO	0000	I 000014	J	000026	JL10	
0007	I 000001	JOUT	0006	000025	JSOL	0006	000031	JSI	0000	I 000017	K	000004	KMAT	
0006	I 000012	L	0003	000004	LANK	0005	I 000463	LLMT	0006	000040	LSAVE	000005	MOL	
0006	000006	MOLES	0000	I 000005	MT	0005	000707	NAME	0006	I 000024	MC	000022	NEWR	
0006	000035	NFZ	0006	000017	NQF	0006	I 000020	NOMIT	0006	000007	NP	000011	NPT	
0006	000027	NREAC	0006	I 000013	NS	0000	I 000000	NSPPI	0006	000010	NT	000635	OF	
0004	I 010150	OMIT	0003	000006	OX	0005	001644	OXF	0005	001363	PECMT	0000	I 000011	PHAZ


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0005 000633 PP 0005 0006 RH 0005 001611 ROP 0005 001612 RM 0005 001976 RTEMP
0005 004064 S 0006 000633 SHOCK 0004 016660 SLN 0006 000004 SP 0004 1 015344 SUB
0005 000001 SUMM 0005 000003 SO 0004 R 016514 TEMP 0005 R 000632 THIGH 0005 001643 TLM
0005 R 000630 TLOW 0005 000627 TM 0005 R 000631 TMID 0006 000002 TP 0005 000002 TT
0005 R 000015 T1 0000 R 000016 T2 0005 000646 VMIN 0006 000003 VOL 0005 000650 VPLS
0005 000652 MP 0001 000001 ZERO

```

SUBROUTINE SEARCH

```

00101 1* C SEARCH TAPE FOR THERMO DATA FOR SPECIES TO BE CONSIDERED 000000
00101 2* C 000000
00101 3* C 000000
00101 4* C 000000
00101 5* C 000000
00103 6* C COMMON /HOLCON/ END GAS, IE, IZERO, LAMK, MOL, OX, ZERO /HOLCON/
00103 7* C COMMON/SPECES/COEF(2,7,150),S(150),EM(150,13),ENLM(150),MO(150) 000000
00103 8* C 1,DELM(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2),SLN(150) 000000
00104 9* C INCLUDE SPECPC 000000
00110 10* C COMMON /MISC/ ENN, SUMM, TT, SO, ATOM(3,101), LLMT(25), BO(25), 000000
00110 11* 1 BOP(25,2), TM, TLOW, TMID, THIGH, PP, OP, SUM, OF, PORAT, 000008
00110 12* 2 HSUBD, AM(2), MPP(2), RM(2), VMIN(2), VPLS(2), BP(2), 000000
00110 13* 3 DATA(25), AMI, CPRI, NAME(25,6), ANUM(25,6), PECUT(25), 000000
00110 14* 4 ENT(25), FAZ(25), RTEMP(25), FO(25), DENSI(25), RHOP, 000000
00110 15* 5 RHNI(25), TLM, QXF(25), ENML, ENMSAVE, ENLSAV 000000
00111 16* C COMMON /INDX/ IDEBUG, CONVG, TP, MP, SP, ISV, MOLES, MP, MT, NPT, L, NS, 000000
00111 17* 1 KNAT IMAT, IQI, NOF, NOMIT, IP, MEHR, IONS, MC, JSOL, JLIK, 000000
00111 18* 2 MREAC, IC, JSI, VOL, SHOCK, IT, NFZ, CALCH, IOSAVE, LSAVE 000000
00112 19* C COMMON /CCC/ GRAPH, JOUT, DEMAND 000000
00112 20* C 000000
00113 21* DIMENSION B(4), DATE(2,3), MT(4), OMIT(3,3) 000000
00113 22* EQUIVALENCE (DATE, EM), (ENLM, OMIT) 000000
00115 23* INTEGER END, GAS, OMIT, PHAZ, SUB 000000
00116 24* LOGICAL NEWR 000000
00116 25* C 000000
00116 26* C CHANGE WHEN CHANGE SPECIES SIZE 000000
00117 27* NSPPI=150 000000
00120 28* NC= 0 000001
00121 29* IX= 0 000002
00122 30* SUB(1,1) = END 000003
00123 31* REMIND 4 000011
00124 32* DO 3 I=1,150 000022
00127 33* DO 3 J=1,L 000022
00132 34* A(I,J) = 0.0 000022
00135 35* READ(4,5) TLOW, TMID, THIGH 000027
00142 36* 5 FORMAT (3F10.3) 000037
00143 37* NS = 1 000037
00144 38* 7 READ (4,10) (SUB(NS,I), I=1,3), DATE(1,NS), DATE(2,NS), (MT(I,J), B(I,J)), 000042
00144 39* 1 J=1,4, PHAZ, T1, T2 000042
00144 40* 10 FORMAT(3A4,6X,2A3,4X(A2,F3.0),A1,2F10.3) 000112
00145 41* IF (SUB(NS,1).EQ.END) GO TO 171 000112
00167 42* READ (4,20) ((COEF(I,J,NS), J=1,7), I=1,2) 000115
00200 43* 20 FORMAT (5E15.8) 000135
00201 44* IF (NOMIT.EQ.0) GO TO 810 000135
00203 45* DO 805 I=1, NOMIT 000137
00204 46* DO 804 I=1, 1 000154

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SEARCH

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00211 47* 804 IF (OMIT(J,I) .NE. SUB(NS,J)) GO TO 805
00214 48* GO TO 7
00215 49* 805 CONTINUE
00217 50* 810 DO 820 K=1,4
00222 51* IF (B(K).EQ.D.) GO TO 825
00224 52* DO 168 I=1,L
00227 53* 168 IF (LLMT(I) .EQ. MT(M)) GO TO 820
00232 54* DO 819 J=1,L
00235 55* 819 A(IJ,NS) = D.
00237 56* GO TO 7
00240 57* 820 A(I,NS) = B(M)
00242 58* 825 IUSE(NS) = D
00243 59* IF (PHAZ.EQ.GAS) GO TO 170
00245 60* NC = NC+1
00246 61* TEMP(MC,1) = T1
00247 62* TEMP(MC,2) = T2
00250 63* IX = IX+1
00251 64* IF IUSE(NS)=1.EQ.D. OR .NC.EQ.11 GO TO 145
00253 65* DO 830 I=1,L
00256 66* 830 IF (A(I,NS) .NE. A,I,NS-1)) GO TO 145
00261 67* IX = IX-1
00262 68* 145 IUSE(NS) = -IX
00263 69* 170 NS = NS+1
00264 70* IF (NS.LE.NSP1) GO TO 7
00266 71* WRITE (JOUT,871)
00270 72* 871 FORMAT (//20X,5#DIMENSIONS IN /SPECIES/ FOUND TO BE TOO SMALL IN S
00270 73* ISEARCH/)
00271 74* 171 NS = NS-1
00272 75* NEWR = .FALSE.
00273 76* WRITE (JOUT,172)
00275 77* 172 FORMAT(42#SPECIES BEING CONSIDERED IN THIS SYSTEM )
00276 78* DO 174 I=1,NS,5
00301 79* K = I + 4
00302 80* 2F (NS.LT. K) K = NS
00304 81* 174 WRITE (JOUT,176) (DATE(I,J),DATE(2,J),SUB(J,1),SUB(J,2),SUB(J,3),
00304 82* 1 J=1,K)
00317 83* 176 FORMAT(5(X,2A3,2X,3A4))
00320 84* CALL MOVABS(500,50)
00321 85* CALL HOLDIT
00322 86* CALL PABIT
00323 87* CALL GOUT(' ',1)
00324 88* RETURN
00325 89* END

```

END OF COMPILATION: NO DIAGNOSTICS.

8HDE.P SHCK

SHCK

AFOR.S SHCK.SHC
HSA E3 -10/15/80 13:07:51 (12.1)

SUBROUTINE SHCK ENTRY POINT 001367

STORAGE USED: CODE(1) 001401; DATA(1) 000263; BLANK COMMON(2) 000000

COMMON BLOCKS:

0003 COMSIS 00000A
0004 HOLCOM 000010
0005 POINTS 000335
0006 SPECES 017106
0007 MISC 001701
0010 DOUBLE 001560
0011 IMDX 000001
0012 PERF 000166
0013 OUPY 000073
0014 CCC 000003

EXTERNAL REFERENCES (BLOCK, NAME)

0015 ROYES
0016 PAGIT
0017 CHRST
0020 GOUT
0021 MEMOF
0022 HCALC
0023 OUT1
0024 OUT2
0025 EOLBRM
0026 SAVE
0027 OUT3
0030 NWMLS
0031 NRMLS
0032 MWDS
0033 NI02S
0034 SORT
0035 NI03S
0036 NI01S
0037 ALO6
0040 EXP
0041 NERR3S

STORAGE ASSIGNMENT (BLOCK, TYPE, RELATIVE LOCATION, NAME)

0000	00143	125F	0001	000211	14L	0001	000011	1456	0001	000221	15L	0001	001001	150L
0000	000165	152F	0001	000022	156G	0000	000101	16F	0001	001112	161L	0001	000126	17L
0001	000143	19L	0001	000073	204G	0001	000114	21L	0001	000136	223G	0001	000147	231G
0001	000245	30L	0001	000356	323G	0001	000376	334G	0001	000520	361G	0001	000534	40L
0001	001125	431L	0001	000320	44L	0001	000325	45L	0000	000137	46F	0001	001057	461G
0001	000412	47L	0001	000547	50L	0001	001201	520G	0001	001232	536G	0001	001247	547G

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SMCK

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0001 001266 5616 0001 001303 5726 0000 000176 58F 0001 001322 6046 0001 001345 6206
0000 000202 68F 0000 000750 75L 0000 000111 61F 0000 000122 622F 0000 000131 633F
0000 000106 880 0006 011052 A 0007 000000 88110 AM 0007 000705 AM1 0007 001135 ANUM
0000 000000 ATMH 0007 000000 ATMH 0000 000036 AX 0000 000037 AX 0000 000024 A1
0000 000034 80 0007 000545 CPH 0000 000036 CALCH 0006 000000 COEF 0011 000001 CONYG
0005 R 000032 CPR 0007 R 000706 CPR1 0007 000634 EPSUM 0007 000654 DATA 0006 010624 DELM
0014 000002 DEMAND 0007 001560 DEMS 0005 R 000064 DLVPT 0005 R 000047 DLVTP 0006 R 004312 EN
0000 000000 END 0006 R 010150 ENLM 0007 001700 ENLSAV 0007 000000 ENM 0007 001676 ENML
0007 001677 ENSAVE 0007 001414 ENTH 0007 000000 EOL 0007 000000 EORAT 0013 000002 FA
0000 000003 FAP 0007 001445 FAZ 0013 R 000005 FB 0013 000006 FC 0000 000007 FCP
0000 000012 FCST 0013 000001 FV 0013 000015 FG 0013 000017 FGE 0013 000020 FGV
0013 000021 FH 0013 000023 FI 0013 000025 FIV 0013 000027 FJM 0000 000001 FMM
0013 R 000031 FMT 0013 R 000030 FM 0013 R 000052 FOUR 0007 000152 FOX 0013 000053 FP
0000 R 000003 FPP 0000 R 000003 FRA 0000 R 000004 FRB 0013 000006 FS 0013 000056 FSV
0013 000057 FT 0013 000061 FTK 0000 R 000005 FTT 0000 R 000006 FU1 0000 R 000007 FU2
0013 000063 FV 0013 R 000065 FVEL 0000 R 000010 FV21 0000 R 000011 FV22 0000 R 000012 FV23
0013 R 000001 F13 0013 R 000000 F9X 0010 D 000000 G 0005 R 000101 GAMMAS 0000 R 000020 GAMMA1
0004 000001 GAS 0010 D 001516 G6 0003 000001 GME1 0014 000000 GRAPH 0011 000003 HP
0007 000692 HPP 0000 R 000030 HS 0007 R 000637 HSUBD 0005 R 000000 HSUM 0006 010376 HO
0000 I 000022 I 0011 000030 IC 0011 I 000000 IDEBUS 0004 000002 IE 0011 000015 IMAT
0000 L 000013 INCDEQ 0000 L 000014 INCOF2 0000 000233 INJPS 0004 I 000021 IOF 0011 000023 IONS
0011 000021 IP 0011 000037 IQSAVE 0011 000016 IO1 0011 I 000005 ISV 0011 000034 IT
0006 I 016266 IUSE 0004 I 000003 IZEPO 0000 I 000025 J 0011 000026 JLIQ 0014 I 000001 JOUT
0011 000025 JSOL 0011 000031 JS1 0000 I 000040 K 0011 000014 KMAT 0004 000004 LAMK
0007 000463 LLMT 0011 000040 LSARE 0012 R 000116 MACH1 0004 000005 MOL 0011 000006 MOLES
0000 R 000017 MU12RT 0000 R 000016 M1 0012 R 000150 M2M1 0007 I 000707 NAME 0011 000024 MC
0011 000022 MEVR 0011 000035 MF2 0011 I 000012 MLM 0011 I 000017 NOF 0011 000020 NMIT
0011 000007 MP 0011 I 000011 MPT 0011 I 000027 MREAC 0011 I 000013 NS 0000 I 000023 NSK
0000 I 000000 MSP1 0011 000010 NT 0007 R 000635 OF 0013 000047 OME 0004 000006 OX
0007 R 001644 OXF 0005 R 000116 P 0003 000002 PAIM 0012 R 000000 PCP 0007 001363 PECMT
0007 R 000633 PP 0005 R 000217 PPP 0000 R 000026 P1 0000 R 000031 P21 0000 R 000033 P211
0003 000003 RBAR 0003 R 000004 RRR 0015 L 000000 RDYES 0007 000644 RH 0007 001611 RMOP
0000 R 000035 RH012 0007 001612 RMV 0012 R 000133 RRHO 0007 R 001476 RTEMP 0003 000005 RVR
0006 004064 S 0000 L 000015 SEQL 0000 000041 SHKIMP 0011 000033 SHOCK 0006 016660 SLM
0005 000251 SONVEL 0011 000004 SP 0005 R 000015 SSUM 0006 015364 SUB 0007 000001 SUMM
0007 000003 SQ 0005 R 000150 T 0006 016514 TEMP 0007 000632 TMIGH 0013 R 000070 THREE
0007 R 001643 TLM 0007 000630 TLOW 0007 000627 TM 0007 000631 TMID 0005 000320 TOTM
0011 L 000002 TP 0007 R 000002 TT 0005 R 000266 TTY 0013 R 000071 TWO 0000 R 000027 T1
0012 R 000047 T21 0000 R 000032 T21 0000 R 000034 T21L 0005 R 000303 UTWO 0012 R 000101 U1
0012 R 000064 U1U2 0005 000202 V 0007 000646 VMIM 0012 000032 VMOC 0011 000032 VOL
0007 000650 VPLS 0005 R 000234 VM 0010 D 001510 X 0004 000007 ZERO
0013 000072 ZEROF

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00101 SUBROUTINE SMCK 000000
00102 1* 2* 3* 4* 5* 6* 7* 8* 9* 10* /CONSTS/ /CONSTS/
00103 00101 000000 /CONSTS/ /CONSTS/
00104 00103 000000 /CONSTS/ /CONSTS/
00105 00104 000000 /CONSTS/ /CONSTS/
00106 00105 000000 /CONSTS/ /CONSTS/
00107 00106 000000 /CONSTS/ /CONSTS/
00108 00107 000000 /CONSTS/ /CONSTS/
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00212 670 21 IOF = IOF+1
00213 680 OF = OFX(IOF)
00214 690 CALL NEWOF
00215 700 INCDEQ = SEQL
00216 710 PP = P(1)
00217 720 II = I(1)
00218 730 IF (INCDEQ) GO TO 19
00219 740 C FROZEN
00220 750 DO 110 I = 1,13
00221 760 DLVTP(I) = 1.0
00222 770 DLVPT(I) = -1.0
00223 780 DO 35 MP1=1,NSX
00224 790 PPP(NPT) = P(NPT)
00225 800 TTT(NPT) = T(NPT)
00226 810 IF (IMPT, EQ, 1) GO TO 14
00227 820 IF (PPP(NPT) - LE, 0.0) PPP(NPT) = PPP(NPT)-1
00228 830 IF (TTT(NPT) - LE, 0.0) TTT(NPT) = TTT(NPT)-1
00229 840 SSUM(NPT) = SSUM(NPT)-1
00230 850 HSUM(NPT) = HSUM(NPT)-1
00231 860 TTT(NPT) = EQ+TT*AND(PPP(NPT), EQ, PP, GO TO 15
00232 870 IF (
00233 880 PP = PPP(NPT)
00234 890 TT = TTT(NPT)
00235 900 CALL MCALC
00236 910 HSUM(NPT) = HSUBN
00237 920 IF (CPRI GT, 0.0) GAMMA1 = CPRI/(CPRI - 1.0/AM1)
00238 930 IF (GAMMA1 GT, 0.0) GO TO 30
00239 940 WRITE(JOUT,16)
00240 950 FORMAT (1/20X,3A)MISSING GAMMA1 OR CP VALUE IN SHCK/)
00241 960 RETURN
00242 970 A1 = SORT(BR0GAMMA1,TT/AM1)
00243 980 IF (U1(NPT) - LE, 0.0) U1(NPT) = A1*MACH1(NPT)
00244 990 IF (MACH1(NPT) - LE, 0.0) MACH1(NPT) = U1(NPT)/A1
00245 1000 WH(NPT) = AM1
00246 1010 CPR(NPT) = CPRI
00247 1020 GAMMA(NPT) = GAMMA1
00248 1030 EOL = .FALSE.
00249 1040 C OUTPUT--ISY CONDITION
00250 1050 WRITE(JOUT,861)
00251 1060 861 FORMAT(M1,43X,39H)INCIDENT SHOCK WAVE PARAMETERS ASSUMING
00252 1070 IF (.NOT. INCDEQ) GO TO 44
00253 1080 WRITE(JOUT,862)
00254 1090 862 FORMAT (11H,51X,25H)EQUILIBRIUM COMPOSITION (/)
00255 1100 GO TO 45
00256 1110 44 WRITE(JOUT,863)
00257 1120 863 FORMAT (11H,53X,18H)FROZEN COMPOSITION (/)
00258 1130 45 CALL OUT1
00259 1140 46 FORMAT (16M) INITIAL GAS (1) )
00260 1150 FMT(3) = F13
00261 1160 FMT(4) = FOUR
00262 1170 WRITE(JOUT,FMT) FN,FB,(MACH1(J), J = 1,NPT)
00263 1180 FMT(4) = TWO
00264 1190 WRITE(JOUT,FMT) FV1,FVEL,(U1(J), J = 1,NPT)
00265 1200 CALL OUT2
00266 1210 BEGIN CALCULATIONS FOR 2ND CONDITION
00267 1220 IF (INCDEQ) EOL = .TRUE.

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ORIGINAL PAGE IS
OF POOR QUALITY

SMCK

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00303 1230      NPT = 1
00304 1240      97 GAMMA1 = GAMMA5(NPT)
00305 1250      M1 = UM(NPT)
00306 1260      P1 = PPP(NPT)
00307 1270      T1 = TTT(NPT)
00308 1280      M5 = MSUM(NPT)
00309 1290      P21 = (2.0 * GAMMA1 * MACH1(NPT) ** 2 - GAMMA1 * 1.1) / (GAMMA1 * 1.1)
00310 1300      T21 = P21 * (2.0 * MACH1(NPT) ** 2 - GAMMA1 * 1.1) / (GAMMA1 * 1.1)
00311 1310      IF (T1 * T21) .GT. 2000. .AND. EQL T21 = .7 * T21 + 600. / T1
00312 1320      MU12RT = AM1 * U1(NPT) ** 2 / (RBR * T1)
00313 1330      P21L = AL06(P21)
00314 1340      T21L = AL06(T21)
00315 1350      DQ 100 I = 1.0
00316 1360      TT = T21 * T1
00317 1370      PP = P21 * P1
00318 1380      IF (.NOT. EQL) GO TO 90
00319 1390      CALL COLORM
00320 1400      GO TO 50
00321 1410      C FROZEN
00322 1420      90 TLM = AL06 (TT)
00323 1430      CALL MCALC
00324 1440      MSUM(NPT) = MSUB0
00325 1450      CPM(NPT) = CPM1
00326 1460      50 RM012 = M1 * U121 / (MUM(NPT) * P21)
00327 1470      GG = RM012 * MU12RT
00328 1480      G11,1) = GG * OLVP(NPT) - TT * CPM(NPT)
00329 1490      G11,2) = GG * OLVP(NPT)
00330 1500      G11,3) = P21 - 1.0 * MU12RT * (RM012 - 1.0)
00331 1510      GG = (U1(NPT) * RM012) ** 2 / RBR
00332 1520      G12,1) = GG * OLVP(NPT) - TT * (OLVP(NPT) - 1.1) / MU(NPT)
00333 1530      G12,2) = GG * OLVP(NPT) - TT * CPM(NPT)
00334 1540      G12,3) = MSUM(NPT) - M5 - U1(NPT) ** 2 * (1.0 - RM012 ** 2) / (2.0 * RBR)
00335 1550      X(1) = G11,1) * G12,2) - G11,2) * G12,1)
00336 1560      X(1) = (G11,3) * G12,2) - G12,3) * G11,2) / X(1)
00337 1570      X(2) = (G11,1) * G12,3) - G12,3) * G11,3) / X(1)
00338 1580      AX = X(1)
00339 1590      AX = X(2)
00340 1600      IF (AX * LT. 0.) AX = -AX
00341 1610      IF (AX * LT. 0.) AX = -AX
00342 1620      IF (AX * GT. 0.) AX = AX
00343 1630      IF (AX * LT. 0.00005) GO TO 150
00344 1640      AX = AX / 4054552
00345 1650      IF (AX * LE. 1.1) GO TO 75
00346 1660      X(1) = X(1) / AX
00347 1670      X(2) = X(2) / AX
00348 1680      75 P21L = P21L * X(1)
00349 1690      T21L = T21L * X(2)
00350 1700      P21 = EXP(P21L)
00351 1710      100 T21 = EXP(T21L)
00352 1720      WRITE(JOUT,125) U1(NPT)
00353 1730      125 FORMAT(125MOD10 NOT CONVERGE FOR U1=F0.2.66M ANSWERS PROBABLY NO
00354 1740      AT RELIABLE, SOLUTION PROBABLY DOES NOT EXIST)
00355 1750      150 RM01(NPT) = 1. / RM012
00356 1760      M2M1(NPT) = UM(NPT) / AM1
00357 1770      PCP(NPT) = P21

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SHCR

DATE 10/50

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00495 1790 IF (NPT .GE. IDEBUG .AND. IDEBUG .NE. 0) WRITE(JOUT,152) 1,721,P21
00496 1800 152 FORMAT(10,I10,M0,=,11,7X,7M2/T1 =,F9.2,7X,7M2/P1 =,F9.2 )
00497 1810 UTHO(NPT) = U1(NPT)*RMH012
00498 1820 U12(NPT) = U1(NPT)-UTHO(NPT)
00499 1830 IF (.NOT.EQL) GO TO 161
00500 1840 DO 880 N=1,N5
00501 1850 IF (IUSE(N).LT.0) GO TO 880
00502 1860 IF (ENLMIK1.GT.-87..AND.ENLMIK1.LT.-87.1 EN(M,NPT), z EXP(ENLMIK1))
00503 1870 880 CONTINUE
00504 1880 GO TO 431
00505 1890 C FROZEN
00506 1900 1A1 PPRIMP11 = PP
00507 1910 TTT(MPT) = T
00508 1920 GAMMA3(NPT) = CPR(NPT)/(Cp(NPT) - 1.0/AM1)
00509 1930 431 ISV = 0
00510 1940 IF (NPT.LT.NSK) ISV=NPT
00511 1950 IF (NPT.EQ.1) ISV=-1
00512 1960 NPT = MPI11
00513 1970 IF (EQL) CALL SAVE
00514 1980 IF (NPT.LE.NSK) GO TO 47
00515 1990 NPT = NSK
00516 2000 C OUTPUT--2ND CONDITION
00517 2010 WRITE(JOUT,50)
00518 2020 50 FORMAT (14HSHOCKED GAS 121 )
00519 2030 FMT14) = TWO
00520 2040 WRITE(JOUT,FMT) FU2,FVEL,UTHO(J),J = 1,MPT)
00521 2050 CALL OUT2
00522 2060 WRITE(JOUT,60)
00523 2070 60 FORMAT (26HINCIDENT SHOCK PARAMETERS )
00524 2080 FMT14) = THREE
00525 2090 WRITE(JOUT,FMT) FPP,FB,FB,(PCP(J), J = 1,MPT)
00526 2100 WRITE(JOUT,FMT) FTT,FB,FB,(T21(J), J = 1,MPT)
00527 2110 FMT14) = FOUR
00528 2120 WRITE(JOUT,FMT) FMM,FB,FB,(M21(J), J = 1,MPT)
00529 2130 WRITE(JOUT,FMT) FRA,FB,FB,(RMO(J), J = 1,MPT)
00530 2140 FMT14) = TWO
00531 2150 WRITE(JOUT,FMT) FV21,FV22,FV23,(U1U2(J), J = 1,MPT)
00532 2160 CALL OUT3
00533 2170 IMCOG = .FALSE.
00534 2180 IF (IMCOF2.AND.EQL) GO TO 17
00535 2190 IF (IOP.LT.NOP) GO TO 21
00536 2200 IP = .FALSE.
00537 2210 DO 999 K = 1,MREAC
00538 2220 999 RTEMP(K) = T(1)
00539 2230 RETURN
00540 2240 END

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END OF COMPILATION:

NO NO DIAGNOSTICS.

AM06,P

THERMP

THEMP

DATE 101500

PAGE 1

AFOR.S THEMP THEMP
MSA E3 -10/15/80-13:07:55 (19.)

SUBROUTINE THEMP ENTRY POINT 000027

STORAGE USED: CODE(1) 000437: DATA(0) 000117: BLANK COMMON(2) 000000

COMMON BLOCKS:

0001 CONSTA 000006
0004 POINTS 000335
0008 MISC 001701
0004 INDX 000041
0007 OUPY 000073
0010 CCC 000003
0011 CFUEL 000002

EXTERNAL REFERENCES (BLOCK, NAME)

0012 NEWOR
0013 EOLARM
0014 MOVARS
0015 HOLDIT
0016 PASIT
0017 GOUT
0020 OUT1
0021 OUT2
0022 OUT3
0023 OUT4
0024 SAVE
0025 MUDUS
0026 MIOZS
0027 MIOIS
0030 NERR3S

STORAGE ASSIGNMENT (BLOCK, TYPE, RELATIVE LOCATION, NAME)

0000	000021	10F	0000	000025	11F	0001	000033	12E	0001	000022	1258	0001	000044	1326
0000	000041	20F	0000	000045	21F	0000	000054	22F	0001	070234	2256	0001	000261	2416
0000	000006	5F	0001	000041	800L	0001	000111	860L	0001	000162	841L	0001	000207	842L
0000	000062	863F	0001	000265	864L	0000	000070	858F	0001	000354	870L	0001	000403	871L
0001	000274	902L	0001	000006	95L	0005	000440	AM	0005	000705	AM1	0005	001135	ANUM
0003	000000	ATNM	0005	000004	ATOM	0005	000514	80	0005	000545	80P	0006	000036	CALCH
0011	R	000000	CF	0006	000001	CONVE	0004	000032	CPR	0005	000704	CPR1	0005	000634
0005	000654	DATA	0010	000002	DEMAND	0005	001560	DEMS	0004	000044	OLVPT	0004	000047	OLVTP
0005	001700	ENLSAV	0005	000000	EMN	0005	001676	EMML	0005	001677	ENSAVE	0005	001414	ENTM
0005	000636	ENRAT	0007	000002	FA	0007	000003	FAP	0005	001445	F42	0007	000005	FB
0007	000006	FC	0007	000007	FCP	0007	000012	FCST	0007	000014	FCV	0007	000015	FG
0007	000017	FEE	0007	000020	F5V	0007	000021	FM	0007	000023	F1	0007	000025	F14
0007	000027	FM	0007	R	000031	FMT	0007	000050	FM	0007	000052	FOUR	0005	001527
0007	000053	FP	0007	000054	S	0007	000056	F5V	0007	000057	F7	0007	000061	FTK
0000	R	000000	FUA	0000	R	000001	FUB	0007	000063	FV	0007	000065	FVEL	0007

0007	000000	FX	000101	GAMMAS	0003	000001	CRZY	0000	000000	GRAPH	0011	000001	MMVU
0005	000003	MP	000442	MPP	0009	R	000437	MSUB	0000	000000	MSUM	0000	I 000003
0004	000003	IC	00004	IDEBUE	0006		000015	IMAT	0000	000100	IMJPS	0000	I 000002
0004	000020	IONS	0006	I 000021	IP	0006	000037	IQSAVE	0006	000016	IOI	0006	I 000005
0006	000034	IT	000026	JLIQ	0010	I 000001	JOUT	0006	000025	J5OL	0006	000031	J5I
0006	000016	KNAT	000043	LLMT	0006	000040	LSAVE	0006	000000	MLERS	0006	000707	NAME
0006	000024	MC	000027	MCWR	0006	000035	MCZ	0006	000012	MLM	0006	I 000017	NOF
0006	000020	MMHIT	0006	I 000007	MP	0006	I 000011	NPT	0006	000027	MREIC	0006	000013
0006	000010	MT	000035	OF	0007	R 000067	ONE	0005	R	000694	OFF	0006	R 000116
0003	000002	PATN	0003	001363	PECWT	0005	R 000633	PP	0004	000217	PPP	0003	R 000003
0003	000004	ADR	0005	000644	RM	0005	001611	RMOP	0004	000212	RMV	0005	001976
0003	000005	ATB	0006	000033	SADCK	0006	000251	YANVAL	0006	000612	RMV	0005	000015
0005	000001	SUMM	0005	000003	SO	0004	R 000150	Y	0005	000004	SP	0006	000070
0005	001643	TLM	0005	000003	TLOW	0005	000627	TM	0005	000632	TMSH	0007	000070
0006	000002	TP	0005	R 000002	TY	0004	000266	TTY	0005	000631	TMIQ	0004	R 000320
0004	000303	VLM	0005	000446	VMIN	0006	L 000032	VOL	0005	000690	VPLS	0004	R 000202
0005	000652	VM	0007	000072	YERO				0005	000690	VPLS	0004	R 000234

10	C	SUBROUTINE	THERP	000000
00101		COMMON /CONS1/	ATM, GMEI, P, IN, ROAD, RDR, RVR	000000
00101	20	COMMON /POINTS, NSUM	(13), SSUM(13), CPR(13), DLVTP(13), DLVPT(13)	000000
00101	30	1 GAMMAS(13), P(26), V(13), PP(13), NM(13)	, SOMVEL(13), TTT(13)	000000
00104	40	2 VLM(13), OTM(13)		000000
00104	70	COMMON /MISC/	ENHES, UMN, TT, SO, ATOM(13, 101), LLMT(25), DD(125),	000000
00105	80	1 DD(25, 2), TM, TLOW, TMIO, TMOM, PP, CP, SUM, OF, EORAT,		000000
00105	90	MSUM, AMRZ, MPPIZ, RMIZ, YRMIZ, APLSIZ, MRIZ,		000000
00105	100	3 DATA(25), RM3, CPR1, NAME(25, 6), ANUM(25, 6), PECMT(25),		000000
00105	110	4 ENTH(25), FAZ(25), ATMP(25), FOX(25), DEMS(25), RMOP,		000000
00105	120	5 RMU(25), TLM, OXF(26), ENML, ENSAVE, ENLSAV		000000
00106	130	COMMON /IMOX/	IDBUG, COMVG, TP, MP, SP, ISV, MOLES, NP, MT, NPT, NLM, NS,	000000
00106	140	1 RMAT, IMAT, IOT, MOP, N, MIT, P, MEVR, IONS, NC, JSOL, JLLIO,		000000
00104	150	2 MREC, IC, J31, VOL, SHOCK, ILMFZ, CALCW, ISSAVE, LSAYE,		000000
00107	160	COMMON /OUPY/	F9H, F13, FA, FAP(12), FB, FC, FCP(13), FST(12), FCV, F6(12),	000000
00107	170	1 F5E, F6V, FM(12), FI(12), FIV(12), FM(12), FMT(15), FM(12), FOUR,		000000
00107	180	2 FPF(12), FSV, FT(12), FTM(12), FV(2), FVEL(12), ONE, THREE,		000000
00107	190	3 TWO, ZERO		000000
00107	200			000000
00110	210	COMMON /CCC/	GRAPH, JOUT, DEMAND	000000
00110	220			000000
00111	230	COMMON /CFUEL/CF, MMVV		000000
00112	240	DATA FUA/GHU CAL//, FUB/GHGRAM /		000000
00115	250	LOGICAL MP, SP, TP, VOL		000000
00115	260			000000
00116	270	IF (T11) LE, 0.01 I11 = 3000.0		000000
00120	280	I0F = 0		000000
00121	290	95 I0F = I0F.1		000000
00122	300	OF = OXF(I0F)		000000
00123	310	CALL MEMOF		000013
00123	320	SET ASSIGNED P OR VOLUME		000013
00124	330	DO 871 IP = 1, NP		000013
00127	340	PP = P(IIP)		000035
00130	350	VLM(NPT) = P(IIP)		000035

TABLE AWW

DATE 101580

2913

00270	92*	NPT = 0		000352
00271	93*	870 NPT = NPT + 1		000354
00272	94*	IF(.NOT. TP) T(1)=TY		000356
00273	95*	IF (P.EQ.1.AND. IT.EQ.1) ISV=-ISV	MOL10037	000362
00274	96*	IF(NY.EQ.1) GO TO 871	12-22	000373
00275	97*	IF(1-TP.NPT) ISV=0	12-22	000376
00300		871 ALL SAVE		000403
00301	98*	GO TO 95		000410
00302	99*	END		000416
00306	100*		MOL10045	

END OF COMPILATION: NO DIAGNOSTICS.

ENDS, P
VAFMT

B-116

VARFAT

2FOR'S VARFMT,VARFMT
HSA E3 -10/15/80-13:07:50 (7,)

SUBROUTINE VARFMT ENTRY POINT 000115

STORAGE USED: CODE(11) 000124; DATA(10) 000023; BLANK COMMON(2) 000000

COMMON BLOCKS:

0001 OUP1 000013

EXTERNAL REFERENCES (BLOCK, NAME)

0004 NERH35

STORAGE ASSIGNMENT (BLOCK, TYPE, RELATIVE LOCATION, NAME)

0001	000006	1146	0001	000046	QOL	0001	000100	451	0003	000002	FA	0003	000003	FAP				
0003	000005	FB	0003	000006	FC	0003	000007	FCB	0003	000012	FCST	0003	000014	FCV				
0000	R	000000	FFOUR	0003	000015	FG	0003	000017	FGE	0003	000020	FGV	0003	000021	FM			
0002	R	000023	FI	0003	000025	FIV	0003	000027	FM	0003	R	000031	FMT	0003	000050	FM		
0000	R	000001	FONE	0003	R	000052	FOUR	0003	000053	FP	0003	000054	FS	0003	000056	FSV		
0003	000057	FT	0000	R	000002	FTHREE	0003	000061	FTK	0000	R	000003	FTWO	0003	000063	FV		
0003	000065	FVEL	0000	R	000004	FZERO	0003	000001	F13	0003	000000	P9X	0000	I	000005	I		
0000	000012	INJPS	0003	R	000067	ONE	0003	R	000070	THREE	0003	R	000071	TWO	0003	R	000072	ZERO

B-117

00101	1*	C	SUBROUTINE VARFMT(V,NPT)	000006
00101	2*			000006
00103	3*		COMMON /OUP1/ F9X,E13,FA,FAP(12),ED,EC,FCP(13),ECST(12),FCN,FG(12), /OUP1/	000006
00103	4*		1 FGE,FGV,FM(2),FI(2),FIV(2),FM(2),FMT(15),FM(2),FOUR, /OUP1/	000006
00103	5*		2 FP,FS(2),FSV,FT(2),FTK(2),FV(2),FVEL(2),ONE,THREE, /OUP1/	000006
00103	6*		3 TWO,ZERO	000006
00103	7*	C		000006
00104	8*		DATA FFOUR/SHF9.4)/,FONE/SHF9.1)/,FTHREE/SHF9.3)/,FTWO/SHF9.2)/,	000006
00104	9*		1 FZERO/SHF9.0)/	000006
00112	10*		DIMENSION V(13)	000006
00112	11*	C		000006
00113	12*		DO 45 I = 1,NPT	000006
00116	13*		IF (I .GE. 13) GO TO 40	000006
00120	14*		FMT(1+2) = FOUR	000012
00121	15*		IF (V(1)) .GE. 10.0) FMT(1+2) = THREE	000014
00123	16*		IF (V(1)) .GE. 100.0) FMT(1+2) = TWO	000022
00125	17*		IF (V(1)) .GE. 1.0E4) FMT(1+2) = ONE	000030
00127	18*		IF (V(1)) .GE. 1.0E6) FMT(1+2) = ZERO	000036
00131	19*		GO TO 45	000044
00132	20*	40	FMT(15) = FFOUR	000046
00133	21*		IF (V(1)) .GE. 10.0) FMT(15) = FTHREE	000047
00135	22*		IF (V(1)) .GE. 100.0) FMT(15) = FTWO	000055
00137	23*		IF (V(1)) .GE. 1.0E4) FMT(15) = FONE	000063

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OF POOR QUALITY

VARFMT

00191	24*	IF (VIII) .GE. 1.0E6) FMT(115) = PZERO	000071
00193	25*	45 CONTINUE	000102
00195	26*	RETURN	000102
00196	27*	END	000123

END OF COMPILATION: NO DIAGNOSTICS.

2 No
21 NO IGNORED - IN CONTROL MODE

2FIN

VARFMT

DATE 101580

PAGE

3

RUNID: LEMIST ACCT: JHPA01R5002: PROJECT: SERVICE IN 208

LOAD 15753 11/0 PUR -1 LEMIST

TIME: SUPS: 00:02:51.912 CBSUPS: 057007923

PU: 00:00:38.729 I/O: 00:01:29.681

CC/ER: 00:00:43.5C1 WAIT: 00:00:00.065

IMAGES READ: 61 PAGES: 118

START: 13:09:06 OCT 15, 1980 FIN: 13:08:01 OCT 15, 1980

THE 1108 (HOST2) WILL BE POWERED OFF NO LATER THAN NOV 15 1980

B-119

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(NO. 07)

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• • • • • UNIVAC 1100 TIME/SHARING EXEC ACCOUNT NUMBER • IMPAD0550021 VER. EW 33RHOST2 SITE • HOST 2

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[illegible]

C

APPENDIX C
SOURCE LISTING OF PROGRAM ELEMENTS
WITHOUT MODIFICATIONS

This is a printout of the Lewis Chemical Equilibrium Program without the modifications necessary for coal gasification data. There have been intermediate changes, principally to make the program an interactive one.

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C

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C-2

ORIGINAL PAGE IS
OF POOR QUALITY

C-3

FOR 5 ULMIS,CPHS,LEWIS-CPHS
 W.A. 11-10/25/79-17:37:57 (9,)

SUBROUTINE CPHS ENTRY POINT 000567

STORAGE USED: CDBL(1) 000003; DATA(0) 000160; BLANK COMMON(2) 000000

COMMON BLOCKS:

0003 SPECIES 01,120
 0004 MISC 001264
 0005 DATA 000004
 0006 LOTH 001201
 0007 CCC 000003

LABEL REFERENCES (BLOCK, NAME)

0010 NAME03
 0011 L1028
 0012 AL06
 0013 L1018
 0014 NAME34

STORAGE ASSIGNMENT (BLOCK, TYPE, RELATIVE LOCATION, NAME)

0001	000031	10L	0001	000207	171G	0001	000217	174G	0001	000043	20L	0001	000351	221G
0001	000062	254G	0001	000065	30L	0001	000067	31L	0001	000157	32L	0000	000041	3333F
0001	000164	40L	0001	000176	60L	0001	000230	70L	0001	000233	80L	0001	000412	87L
0001	000060	64F	0001	000472	69L	0001	000531	90L	0000	000103	904F	0000	006034	A
0004	000570	AM	0004	000624	AM1	0004	000741	ANUM	0004	000004	ATOM	0004	000502	B0
0004	000521	00P	0005	000036	CALCH	0003	000000	COEF	0005	000001	CONVG	0006	R 000361	CPL
0004	000625	CPM1	0004	R 000564	CPSUM	0000	R 000040	CPUSED	0000	R 000035	CPX	0000	R 000007	CPXX
0004	000604	DATA	0003	005670	DELN	0007	000002	DEMAND	0004	001167	UENS	0003	R 002734	EN
0001	005360	ENLN	0004	001263	ENLSAV	0004	000000	ENN	0004	001261	ENML	0004	001262	ENSAVE
0001	001073	ENTH	0004	000566	ECHAT	0004	001112	FAZ	0004	001150	FOX	0007	000000	GRAPH
0006	R 000551	HL	0005	000003	HF	0004	000572	HPP	0004	000567	HSURU	0000	R 000034	HX
0000	R 000013	HXX	0003	R 005524	HC	0000	I 000037	I	0005	000030	IC	0005	000000	IDEBUG
0000	I 000001	IEH	0000	I 000023	IENTND	0006	I 001131	ILSP	0005	000015	IMAT	0000	I 000002	IMSG
0000	000132	INJF3	0005	000023	ION5	0005	000021	IP	0005	000037	IOSAVE	0005	000016	IOI
0005	000025	ISV	0005	000034	IT	0003	I 011444	IOSE	0000	I 000026	IX	0005	I 000031	J
0005	000026	JL10	0007	I 000001	JOUT	0005	000025	J5UL	0000	I 000024	K	0000	I 000025	KK
0005	000014	KMAT	0000	I 000027	KX	0004	000463	LLMY	0005	000040	LSAVL	0000	I 000036	M
0005	000006	MEL5	0004	000626	NAME	0005	000024	NC	0005	000022	NEWP	0005	000035	NFZ
0005	000012	NLM	0006	I 000000	NLTSP	0005	000017	NOF	0005	000020	NOM11	0005	000007	NP
0005	I 000011	NPI	0005	000027	NPEAC	0005	I 000013	NS	0000	I 000000	NSPP1	0005	000010	NT
0000	I 000030	NTUP	0004	000565	OF	0004	001227	OXF	0004	001054	PECM1	0004	000563	PP
0004	000574	RE	0004	001206	RHOP	0004	001207	RHW	0004	001131	RTEMP	0003	M 002570	S
0004	000633	SHOCH	0006	K 000741	SL	0003	011754	SLN	0005	000004	SP	0003	I 010770	SUH
0004	I 000001	SHELT	0004	000001	SUMN	0000	R 000033	SX	0000	R 000017	SXX	0004	000003	SD
0001	011610	TIMP	0004	000562	TMIGH	0006	R 000171	TL	0004	R 001226	TLN	0000	R 000032	TLNS
0004	R 000567	TLON	0004	000557	TP	0004	R 000561	TMID	0005	000002	TF	0004	R 000002	TT
0001	R 000031	TTS	0000	R 000033	TXK	0004	000576	VMIN	0005	000032	VOL	0004	000600	VPLS

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C-7

C-7

0006	0005A6	LGRAT	0011	000002	FA	0011	000003	FAP	0006	0011Z	FAZ	0011	R	000005	FR			
0011	000006	FC	0011	R	000007	FCP	0011	000012	FCST	0011	000014	FCV	0011	R	000015	FG		
0011	000017	FGL	0011	000020	FGL	0000	R	000009	FGI	0011	R	000021	FHM	0011	R	000023	FI	
0011	000025	FIV	0011	P	000027	FH	0000	R	000001	FMM	0011	R	000031	FMT	0011	R	000050	FN
0011	000031	FIV	0006	000150	FOX	0011	000053	FP	0000	R	C00003	FPP	0000	R	C00002	FP1		
0011	000052	FJOP	0006	R	000005	FJB	0011	000054	FS	0011	R	000056	FSV	0011	R	000057	FT	
0011	000004	FRA	0000	R	000006	FII	0000	R	000007	FJO	0011	000063	FV	0011	R	000065	FVEL	
0011	000061	FIS	0011	000000	FJK	0000	R	000014	GAM	0005	R	000101	GAMHAS	0006	R	000001	GAS	
0011	000001	FIS	0011	000000	FJK	0000	R	000014	GAM	0005	R	000101	GAMHAS	0006	R	000001	GAS	
0011	000001	GMLT	0010	R	000150	GMI	0012	000000	GRAPH	0007	L	000003	HP	0006	R	000572	HPP	
0011	000567	HSGRO	0005	R	000002	HSMH	0010	M	000064	H1	0007	000030	IC	0007	I	000000	IDERUS	
0011	000002	IF	0000	I	000011	II	0007	000015	IMAT	0007	000143	INJP	S	0007	I	000010	IOF	
0011	000023	IONS	0007	I	000021	IP	0007	000037	IQSAVE	0007	000016	IQI	IT	0007	I	000034	IT	
0011	000012	ITA	0006	I	000003	IZERO	0000	I	000034	J	0007	0~0026	JLIQ	0012	I	000001	JOYT	
0011	000025	JSLM	0007	000031	JSI	0007	000005	K	0007	I	000005	K	LAKE	0006	I	000004	LAKH	
0011	000043	JLMT	0007	000040	LSAVE	0007	000005	MOL	0007	000006	MOLES	NAME	NAME	0006	I	000626	NAMP	
0011	000024	NC	0007	000022	NEWB	0007	000035	MFZ	0007	000012	NLM	NOS	NOS	0007	I	000017	NOS	
0011	000010	NT	0006	I	000007	NP	0007	I	000011	NPT	0007	I	000027	NREAL	0007	R	000013	NS
0011	000010	NT	0006	R	000565	OF	0006	R	000067	ONE	0006	000006	OK	0006	R	001227	OFF	
0011	000016	P	0003	R	000002	PATM	0010	R	000000	PCP	0006	001054	PECHI	0006	R	000563	PP	
0011	000017	PPP	0000	R	000013	PGI	0010	R	000101	PUB	0003	R	000003	RBAR	0003	R	000004	RBP
0011	000054	RH	0006	R	001206	RHQF	0000	R	000020	RK	0006	001207	RMW	0010	R	000047	RWHO	
0011	000021	RPI	0006	R	001131	RTEHP	0003	R	000005	RVR	0007	000033	SHOCK	0005	R	000251	SONVEL	
0011	000004	SP	0005	000015	SSUM	0006	000001	SUMN	0006	000003	SU	0006	000003	T	0005	R	000157	T
0011	000016	TEM	0006	000562	THIGH	0011	R	000070	THREE	0011	001226	TLM	TLOW	0006	R	000560	TLOW	
0011	000057	TM	0006	000561	TMID	0005	000320	TOTN	0007	L	000002	TP	TT	0006	R	000002	TT	
0011	000046	TTT	0000	P	000015	TTI	0010	R	000116	TUB	0011	R	000071	TWO	0000	R		

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000732	000733	000734	000735	000736	000737	000738	000739	000740	000741	000742	000743	000744	000745	000746	000747	000748	000749	000750	000751	000752	000753	000754	000755	000756	000757	000758	000759	000760	000761	000762	000763	000764	000765	000766	000767	000768	000769	000770	000771	000772	000773	000774	000775	000776	000777	000778	000779	000780	000781	000782	000783	000784	000785	000786	000787	000788	000789	000790	000791	000792	000793	000794	000795	000796	000797	000798	000799	000800	000801	000802	000803	000804	000805	000806	000807	000808	000809	000810	000811	000812	000813	000814	000815	000816	000817	000818	000819	000820	000821	000822	000823	000824	000825	000826	000827	000828	000829	000830	000831	000832	000833	000834	000835	000836	000837	000838	000839	000840	000841	000842	000843	000844	000845	000846	000847	000848	000849	000850	000851	000852	000853	000854	000855	000856	000857	000858	000859	000860	000861	000862	000863	000864	000865	000866	000867	000868	000869	000870	000871	000872	000873	000874	000875	000876	000877	000878	000879	000880	000881	000882	000883	000884	000885	000886	000887	000888	000889	000890	000891	000892	000893	000894	000895	000896	000897	000898	000899	000900	000901	000902	000903	000904	000905	000906	000907	000908	000909	000910	000911	000912	000913	000914	000915	000916	000917	000918	000919	000920	000921	000922	000923	000924	000925	000926	000927	000928	000929	000930	000931	000932	000933	000934	000935	000936	000937	000938	000939	000940	000941	000942	000943	000944	000945	000946	000947	000948	000949	000950	000951	000952	000953	000954	000955	000956	000957	000958	000959	000960	000961	000962	000963	000964	000965	000966	000967	000968	000969	000970	000971	000972	000973	000974	000975	000976	000977	000978	000979	000980	000981	000982	000983	000984	000985	000986	000987	000988	000989	000990	000991	000992	000993	000994	000995	000996	000997	000998	000999	001000	001001	001002	001003	001004	001005	001006	001007	001008	001009	001010	001011	001012	001013	001014	001015	001016	001017	001018	001019	001020	001021	001022	001023	001024	001025	001026	001027	001028	001029	001030	001031	001032	001033	001034	001035	001036	001037	001038	001039	001040	001041	001042	001043	001044	001045	001046	001047	001048	001049	001050	001051	001052	001053	001054	001055	001056	001057	001058	001059	001060	001061	001062	001063	001064	001065	001066	001067	001068	001069	001070	001071	00107
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FM1(4) = THREE
WRITEL(JOUT,FMT) FM,FB,(V(J), J = 1,NPT)
FM1(4) = FOUR
WRITEL(JOUT,FMT) FCP,(CP(J), J = 1,NPT)
WRITEL(JOUT,FMT) FGL,FB,FB,(GMI(J), J = 1,NPT)
FM1(4) = ONE
WRITEL(JOUT,FMT) FS,FVEL,(SONVEL(J), J = 1,NPT)
WRITEL(JOUT,SB)
FM1(3) = ONE
CALL OUT2
58 FORMAT(11HORDERED GAS//)
WRITEL(JOUT,SB)
68 FORMAT(22HDETUNATION PARAMETERS //)
FM1(4) = THREE
DO 70 J = 1,NPT
V(J) = PPL(J)/PUB(J)
PCP(J) = TTT(J)/TUB(J)
SONVEL(J) = SONVEL(J)*RRHO(J)
WRITEL(JOUT,FMT) FPP,FB,FB,(V(J), J = 1,NPT)
WRITEL(JOUT,FMT) FTT,FB,FB,(PCP(J), J = 1,NPT)
DO 73 J = 1,NPT
V(J) = WM(J)/ZMI
FM1(4) = FOUR
WRITEL(JOUT,FMT) FMM,FB,FB,(V(J), J = 1,NPT)
WRITEL(JOUT,FMT) FRA,FB,FB,(RPHO(J), J = 1,NPT)
WRITEL(JOUT,FMT) FM,FB,(VMOC(J), J = 1,NPT)
FM1(4) = ONE
WRITEL(JOUT,FMT) FUU,FVEL,(SONVEL(J), J = 1,NPT)
EQL=.TRUE.
CALL OUT3
IF (K.EQ.0 .AND. IOF.EQ. NOF) GO TO 1000
IDEBUG = IDEBUG-13
WRITEL(JOUT,SB)
668 FORMAT(1H)
NPT = 0
670 NPT = NPT + 1
IF (K.EQ.1) K = -1
CALL SAVE
WRITEL(JOUT,SB)
902 CONTINUE
IF (IOF.GE.NOF) GO TO 1000
IDEBUG = IDEBUG+13
GO TO 7
1000 IF = .FALSE.
RETURN
END

```

0.03374	136
0.03375	137.0
0.03405	138.0
0.03406	139.0
0.03415	140.0
0.03426	141.0
0.03437	142.0
0.03447	143.0
0.03451	144.0
0.03462	145.0
0.03463	146.0
0.03464	147.0
0.03466	148.0
0.03467	149.0
0.03468	150.0
0.03469	151.0
0.03470	152.0
0.03471	153.0
0.03472	154.0
0.03473	155.0
0.03474	156.0
0.03475	157.0
0.03476	158.0
0.03477	159.0
0.03478	160.0
0.03479	161.0
0.03480	162.0
0.03481	163.0
0.03482	164.0
0.03483	165.0
0.03484	166.0
0.03485	167.0
0.03486	168.0
0.03487	169.0
0.03488	170.0
0.03489	171.0
0.03490	172.0
0.03491	173.0
0.03492	174.0
0.03493	175.0
0.03494	176.0
0.03495	177.0
0.03496	178.0
0.03497	179.0
0.03498	180.0
0.03499	181.0

ORIGINAL PAGE IS
OF POOR QUALITY

FORM 5 LEMIS-FOURM-LEWIS-LELPHM
 000000 10/25/79-17:38:12 199

SUPROUTINE LULBHM ENTRY POINT 003112

STORAGE USED: 000111 003110; DATA(0) 000440; BLANK COMMON(2) 000000

COMMON BLOCKS:

0003 CONSTS 000006
 0004 MULLON 000010
 0005 POINTS 000035
 0006 SPELCS 01-120
 0007 MISC 001264
 0010 DOUBLE 001560
 0011 IADA 000041
 0012 PLKF 000166
 0013 CCC 000003

EXTERNAL REFERENCES (BLOCK, NAME)

0014 CPHJ
 0015 MATHIA
 0016 GAUSS
 0017 ALOC
 0018 N=0001
 0019 7,1018
 0020 7,1023
 0021 EXP
 0022 NERH35

STORAGE ASSIGNMENT (BLOCK, TYPE, RELATIVE LOCATION, NAME)

0001	001402	100L	0001	001211	101L	0001	002164	10236	0001	002214	10336	0000	000201	110F
0001	001452	111L	0001	001575	1115L	0001	001633	1116L	0001	001517	113L	0001	002475	11306
0001	002503	11346	0001	001513	114L	0001	001542	115L	0001	002543	11506	0001	001660	116L
0001	002616	1160L	0001	002446	1165L	0001	002710	1171L	0000	000202	1183F	0001	002636	12016
0001	002676	12176	0001	002733	12406	0001	002046	13L	0001	001747	130L	0000	000300	136F
0001	002652	143L	0000	000236	144F	0001	002255	147L	0001	002262	148L	0001	000116	1516
0001	002710	153L	0001	002304	154L	0000	000244	156F	0001	002334	157L	0001	002373	158L
0001	002831	159L	0001	002144	160L	0000	000256	161F	0001	000151	1656	0001	002622	165L
0001	002842	166L	0000	000266	168F	0001	002610	169L	0001	002613	170L	0001	002717	171L
0001	002877	172F	0001	000430	174L	0001	002002	183L	0001	003005	186L	0000	000153	1924F
0001	002774	199L	0000	000305	201F	0001	001561	2115L	0001	000244	2216	0001	000277	2326
0001	000000	244F	0001	000325	2456	0001	000332	2516	0001	000374	2706	0001	000406	2776
0001	000000	306F	0001	000464	3156	0001	000517	3246	0001	000131	33L	0001	000613	3606
0001	000071	373F	0001	002645	40L	0001	000721	4166	0001	000732	4226	0001	000155	44L
0001	001013	4456	0001	001141	4776	0001	000125	499L	0001	001172	5066	0001	001252	5316
0001	001413	600F	0001	001313	62L	0001	000251	63L	0001	001464	6316	0001	000302	67L
0001	001423	6736	0001	001642	7046	0001	000342	72L	0001	001722	7266	0000	000075	73F
0001	000426	74F	0001	001760	7466	0000	000303	771F	0000	000063	772F	0001	000412	773L
0001	000224	774L	0001	001936	775L	0000	000132	776F	0001	000747	80L	0001	000766	83L


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0001 001023 04L 0001 001036 85L 0001 000571 871L 0001 003063 873L 0000 000105 874F
0001 001332 917L 0000 000134 923F 0000 000157 924F 0000 000176 925F 0001 000603 966L
0001 000622 968L 0001 000632 969L 0001 001111 97L 0001 000635 970L 0001 000644 971L
0000 000220 973F 0001 000654 997L 0006 R 0006034 A 0000 R 000047 AA 0012 000150 AEA1
0007 000570 AM 0000 R 000042 AMBA 0007 000043 AMBDA1 0007 R 000624 AM1 0007 000741 ANUM
0011 000133 APP 0003 000000 ATMN 0007 000004 ATOM 0005 R 000032 CPR1 0007 000521 BOP
0006 000036 CALCH 0006 000000 COF1 0007 000604 DATA 0005 R 000055 DELF 0007 000625 DELH
0013 000002 DEMAND 0007 R 000026 CH1V 0007 000001 CONVG 0005 R 000064 DLPV1 0006 R 000670 DELH
0006 R 002734 LN 0004 000000 END 0000 R 000025 ENL 0005 R 000001 GAS 0005 R 000047 DLTVP
0007 R 000000 ENN 0007 R 001261 ENN1 0006 R 005360 ENLW 0007 001263 ENLSAV
0012 000165 EUL 0007 R 000566 EORAT 0007 001262 ENSAVE 0000 R 000033 ENSOL 0007 001073 ENTH
0010 00150 FOX 0010 000000 G 0005 R 000101 GAMMAS 0004 000001 GEG1 0000 R 000046 FNEG2
0011 000000 GRAPH 0011 L 000003 HP 0007 000572 HPP 0007 000567 HSUBU 0003 000001 GMET
0005 R 005524 HO 0000 000032 I 0011 L 000030 IC 0007 000572 HPP 0007 000567 HSUBU 0003 000001 GMET
0011 000015 IMAT 0000 000051 INC 0000 000400 INJPS 0011 000000 IOERUG 0005 R 000000 HSUM
0011 000037 IQSAVE 0011 000016 IQ1 0000 000035 IQ2 0000 L 000022 ISING 0011 000021 IP
0011 000034 IT 0000 000030 ITNUMR 0006 0011444 JK6 0004 000003 IZER0 0011 000005 ISV
0000 000056 JOELF 0000 000037 JJ 0000 000053 JKG 0004 000003 IZER0 0011 000005 ISV
0011 000025 JSOL 0011 000031 JS1 0000 000052 KG 0011 000026 JLIQ 0013 000001 JOUT
0004 000004 LANK 0007 000463 LLMT 0000 000023 LOGV 0011 000014 KMAT 0011 000012 L
0011 000006 MOLES 0007 000626 NAME 0011 000024 NC 0000 000040 LSAVE 0004 000005 MOL
0011 000035 MZ 0011 000017 NOF 0011 000020 NOMIT 0011 000007 NP 0011 000011 NPI
0011 000027 NREAC 0011 000013 NS 0000 000000 NSPPI 0011 000010 NT 0000 000036 NTZERO
0000 000034 NMR 0007 000565 OF 0004 000006 OX 0007 001227 OXF 0005 000116 P
0001 000002 PAIM 0012 000000 PCP 0003 000004 RBR 0007 000563 PP 0007 001206 RHOP
0000 000001 PLOW 0003 000003 RBR 0007 000563 PP 0007 001206 RHOP
0010 L 000024 RTE 0007 001207 RMW 0007 001131 RTEMP 0003 R 000005 RVR 0006 R 002570 S
0011 L 000033 SHOCK 0000 R 000027 SIZEF 0006 0011754 SLN 0005 000251 SONVEL 0012 000101 SUBAR
0012 000047 SPIM 0000 R 000050 S5 0000 R 000015 SUM 0012 000116 SUPAR 0007 R 000003 SO
0000 000020 SUM 0007 R 000001 SUMN 0000 R 000044 SUM1 0007 R 000562 THIGH 0007 R 000560 TLOW
0005 R 000150 T 0006 R 001610 TEMP 0007 000561 TMID 0000 R 000057 TN 0005 R 000320 TOTN
0007 R 000557 T* 0000 R 000054 THELT 0005 R 000266 TTT 0005 000202 V 0012 000064 VAC1
0011 L 000002 TP 0007 R 000002 TT 0012 000032 VMOC 0011 000032 VOL 0007 000600 VPLS
0005 R 000503 VLM 0007 000576 VMIN 0010 001510 X 0004 000007 ZERO
0007 R 000234 WM

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SUBROUTINE EQUILBRM
C ROUTINE TO CALCULATE EQUILIBRIUM COMPOSITION AND PROPERTIES
COMMON /CONSTS/ ATMN,GMET,PAIM,RBAR,RBR,RVR
COMMON /HOLCON/ ENL,GAS,IE,IZERO,LANK,MOL,OX,ZERO
COMMON /POINTS/SSUM(13),SSUM(13),CPR(13),ULVTP(13),ULVTP(13),ULVTP(13)
1 .GAMMAS(13),P(26),I(26),V(13),PP(13),MM(13),SONVEL(13),T(13)
2 .VLM(13),TOTN(13)
COMMON /SPECES/COEF(2,7,150),SI(150),EN(150,13),ENL(150),H(150)
1 .DELN(150),AT(5,150),SUB(150,3),IUSL(150),TEMP(150,2),S(150)
INCLUDE SPELCPH
COMMON /MISC/ ENL,SUM,AT,SI,ATOM(3,101),LMT(15),H(15),
1 .UP(15,2),TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EURAT,
2 .MSUB,AM(2),HPP(2),PH(2),VMIN(2),VPLS(2),WP(2),
3 .DATA(16),AM1,CPR1,NAM(15,3),ANUM(15,5),FECA(15),
1301 19
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000000 /MISC/
000000 /MISC/
000000 EQNM0013
000000 /INUM/
000000 /INUM/
000000 /INUM/
000000 /PERF/
000000 /PERF/
000000 /PERF/

1 ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENST(15),PHOP,
2 RMV(15),ILN,ORF(26),ENNL,ENSAVE,ENLSAV
3 COMMON /DOUBLE/ G(20,21), X(20)
4 COMMON /INUMX/ IDBUG,CONVG,TP,MP,SP,ISV,MOLES,NP,NT,NPT,L,NS,
5 KMAT,IMAT,IQI,NOF,NOMIT,IP,NEWR,IONS,NC,JOL,JLIO,
6 NPEAC,IC,JSI,VOL,SHOCK,IT,IMPZ,CALCH,IOSAVE,LSAVE
7 COMMON /PERF/ PCP(24),VMOC(13),SPIM(13),VACI(13),SUBAR(13),
8 SUPAR(13),APP(13),AEAT(13),EVL
9
10 COMMON /CCC/ GRAPH,JOUT,DEMAND
11
12 DIMENSION PROM(15)
13 DOUBLE PRECISION G,SUM,X
14 LOGICAL CONVG,MP,IC,IONS,ISING,LOGV,RITE,SHOCK,SP,TP,VOL
15
16 ENL = ENNL
17 RITE = .FALSE.
18 IF (IDBUG.GT.0.AND.NPT.GE.IDEBUG) RITE=.TRUE.
19 CHIV = 5.0E-6
20 SIZEF = 0.
21 ISING = .FALSE.
22 LOGV = .FALSE.
23 IF (VOL) PP = RVROENN*TT/VLM(NPT)
24 TLN = ALOG(11)
25 CONVG = .FALSE.
26 ITNUMB = 100
27 JSI = 1
28 CALL CPHS
29 TM = ALOG(PP/ENNI)
30 IF (IC) PREVIOUS POINT HAD SINGULAR MATRIX
31 IF (IC) GO TO 966
32 IF (.NOT.IONS.OR.IE.EQ.LLMT(1)) GO TO 33
33 L = L+1
34 ICI = 101*1
35 DO 499 J = 1,NS
36 IF (AL(J).EQ.0.) GO TO 499
37 EN(J,NPT) = 1-E-R
38 ENL(NJ) = -R*4206810
39 TUSE(J) = 0
40
41 499 CONTINUE
42 IF (INPT.EQ.1.AND..NOT.SHOCK) WRITE(JOUT,244)(LLMT(I),I=1,L)
43 244 FORMAT (40PT,14(5X,A4))
44 BEGIN ITERATION
45 IF (IC) GO TO 1171
46 SUMS = ENN
47 IF (JSOL.EQ.0) GO TO 6.
48 ENSOL = EN(JSOL,NPT)
49 EN(JSOL,NPT) = EN(JSOL,NPT)+EN(JLIO,NPT)
50 TUSE(JLIO) = -TUSE(JLIO)
51 I-1 = ICI-1
52 OLVT(NPT) = 0.
53 LFN(NPT) = 0.
54 GAMMA5(NPT) = 0.
55 LOGV = .TRUE.
56 CALL MATRIX
57
58 1171
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65 1180
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[illegible]

C-15


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EQLNU080
EQLNU081

EQLNU084

EQLNU089
EQLNU090

EQLNU096
EQLNU099
EQLNU100
EQLNU101

EQLNU104
EQLNU105
EQLNU106

00 99 I = 1, L
99 UELN(J) = DELN(J) * A(I, J) * X(I)
GO TO 101
100 UELN(J) = X(J)
JJ = JJ + 1
101 CONTINUE
AMBDAL = 1.
AMBDAL = 1.
SUM = X(I)
IF (SUM, LT, 0.) SUM = -SUM
IF (OLNT, GT, SUM) SUM = OLNT
IF (OLNT, GT, SUM) SUM = -OLNT
00 917 J = 1, NS
IF (IUSC(J), NE, 0) GO TO 917
IF (LEN(J, NPT)) * GT, 0.0 * AND, DELN(J) * GT, SUM SUM = DELN(J)
IF (LEN(J, NPT)) * GT, 0.0 * OR, UELN(J) * LE, 0.0 GO TO 917
SUM = (-9.212 - ENLN(J)) * ENL / (DELN(J) - X(I))
IF (SUM, LT, 0.) SUM = -SUM
IF (SUM, LT, AMBDAL) AMBDAL = SUM
917 CONTINUE
IF (SUM, GT, 2. * AMBDAL) SUM = 2. / SUM
IF (AMBDAL, LT, AMBDAL) AMBDAL = AMBDAL
IF (NOT, RITE) GO TO 111
WRITE(JOUT, 923) IT, ENN, ENL, PP, IM, AMBDA
923 FORMAT (3HUT, E15.8, 6H ENN, E15.8, 7H ENL, E15.8, 5H PP, E15.8,
1 9H LN P, N, E15.8, 8H AMBDA, E15.8)
IF (VOL) WRITE(JOUT, 1924) VLM(NPT)
1924 FORMAT (4H VOLUME, E15.8, 2HCC)
924 FORMAT (1H0, 18X, 2HNI, 12X, 5HLN NI, 8X, 9HDEL LN NI, 10X, 4HHR/RT, 9X, 4HSD/
1H, 12X, 6H-GO/RT, 9X, 5H-G/RT)
00 926 J = 1, NS
FNEG1 = S(J) - H(J)
FNEG2 = FNEG1
IF (IUSE(J), EG, 0) FNEG2 = FNEG2 - ENLN(J) - IM
926 WRITE(JOUT, 925) SUB(J, 1), SUB(J, 2), SUB(J, 3), EN(J, NPT), ENLN(J),
UELN(J), H(J), S(J), FNEG1, FNEG2
A
925 FORMAT (1X, 34X, 7E15.6)
WRITE(JOUT, 110)
110 FORMAT (1H0)
L APPLY CORRECTIONS TO ESTIMATES
111 SUM = 0.
00 113 J = 1, NS
IF (IUSE(J)) 113, 112, 114
112 ENLN(J) = ENLN(J) * AMBDA * DELN(J)
EN(J, NPT) = 0.
IF (LEN(J) * 18.4206810 * LE, ENL) GO TO 113
EN(J, NPT) = EXP(ENLN(J))
SUM = SUM + EN(J, NPT)
GO TO 113
114 EN(J, NPT) = EN(J, NPT) * AMBDA * DELN(J)
113 CONTINUE
SUM = SUM
IF (ITP) GO TO 115
ITP = ITP * AMBDAL * ENL
IT = EXP(ITP)

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10055 2416 JSI = 1
10056 2420 CALL CMHS
10057 2430 115 IF (VUL) GO TO 2115
10058 2440 ENL = LNL*AMBOA*(1Q1)
10059 2450 ENN = EXP(ENL)
10060 2460 GO TO 1115
10061 2470 2115 ENN = SUMN
10062 2480 LNNL = ALOG(ENN)
10063 2490 PP = EXP(OT*ENN/VLM(NPT))
10064 2500 1115 TM = ALOG(PP/ENN)
10065 2510 IF (CLM(TL)*NE,IE) GO TO 116
10066 2520 C CHECK ON REMOVING IONS
10067 2530 DO 1116 J = 1,NS
10068 2540 IF (AIL(J)*EQ,0.) GO TO 1116
10069 2550 IF (ENL(NPT)*GT,0.) GO TO 116
10070 2560 1116 CONTINUE
10071 2570 DO 1118 J=1,NS
10072 2580 1118 IF (AIL(J)*NE, 0.0) IUSE(J) = - 10000
10073 2590 L = L-1
10074 2600 101 = 101-1
10075 2610 GO TO 43
10076 2620 C TEST FOR CONVERGENCE
10077 2630 116 IF (ITNUM-EQ,0) GO TO 13
10078 2640 IF (AMODA-LI,1.) GO TO 43
10079 2650 SUM = ITNN-SUMN/ENN
10080 2660 IF (SUM,LT,0.) SUM = -SUM
10081 2670 IF (SUM*GT, CHITV) GO TO 43
10082 2680 DO 130 J=1,NS
10083 2690 IF (IUSE(J)*LT,0) GO TO 130
10084 2700 AA = UENL(J)/SUMN
10085 2710 IF (AA*LT,0.) AA = -AA
10086 2720 IF (IUSE(J)*EQ,0) AA = AA*ENL(J,NPT)
10087 2730 IF (AA*GT, CHITV) GO TO 43
10088 2740 130 CONTINUE
10089 2750 C CALCULATE ENTROPY, CHECK ON UELTA S FOR SP PROBLEMS
10090 2760 TOTN(NPT) = 0.
10091 2770 SSUM(NPT) = 0.
10092 2780 DO 183 J=1,NS
10093 2790 IF (IUSE(J)*LT,0) GO TO 183
10094 2800 TOTN(NPT) = TOTN(NPT) + ENL(J,NPT)
10095 2810 SS = SS+J
10096 2820 IF (IUSE(J)*EQ,0) SS=SS-ENL(J,NPT)
10097 2830 SSUM(NPT) = SSUM(NPT)+SS*ENL(J,NPT)
10098 2840 183 CONTINUE
10099 2850 IF (NCT,SE,OF,NPT,EQ,1) GO TO 13
10100 2860 SS = SSUM(NPT) -SS
10101 2870 IF (SS*LT,-0.00005).OR,SS*GT,0.00005) GO TO 43
10102 2880 IF (ITL)*RTLE(JOUT,1183) SS
10103 2890 1183 FORMAT(1,HURELTA 5/R =,E15.4)
10104 2900 13 CONVER = TRUE.
10105 2910 IF (ITL)*TL,LOW,OF,11)*GT,1HIGHWRITELJOUT,306,IT,NPT
10106 2920 306 FORMAT(7H)TIME TEMPERATURE=E12.4,26H IS OUT OF RANGE FOR POINT,15HRELNU119
10107 2930 IF (ITL)*B,M,N) GO TO 160
10108 2940 *RTLE(JOUT,973) NPT
10109 2950 977 FORMAT (75A,4H)100 ITERATIONS DID NOT SATISFY THE CONVERGENCE REQ
10110 2960 1016MENTS FOR POINT,137)

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EQLNU110
EQLNU112
EQLNU113

EQLNU115

EQLNU133

EQLNU136

EQLNU117

[illegible]

6.10.10	2.97.7
6.10.12	2.98.8
6.10.14	2.99.9
6.10.15	300.0
6.10.16	301.1
6.10.16	302.2
6.10.16	303.3
6.10.21	304.4
6.10.22	305.5
6.10.25	306.6
6.10.27	307.7
6.10.30	308.8
6.10.33	309.9
6.10.35	310.0
6.10.39	311.1
6.10.41	312.2
6.10.42	313.3
6.10.42	314.4
6.10.43	315.5
6.10.49	316.6
6.10.55	317.7
6.10.55	318.8
6.10.57	319.9
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6.10.68	322.2
6.10.65	323.3
6.10.67	324.4
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6.10.73	327.7
6.10.75	328.8
6.10.77	329.9
6.10.80	330.0
6.10.82	331.1
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6.10.84	333.3
6.10.86	334.4
6.10.86	335.5
6.10.87	336.6
6.10.88	337.7
6.10.89	338.8
6.10.91	339.9
6.10.92	340.0
6.10.92	341.1
6.10.92	342.2
6.10.92	343.3
6.10.92	344.4
6.10.92	345.5
6.10.92	346.6
6.10.92	347.7
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6.10.92	352.2

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FOR S L L S FROZEN, LEWIS, FROZEN
 N/A 13-10/25/79-17:38:28 (8.1)

SUBROUTINE FROZEN ENTRY POINT 000345

STORAGE USED: C001(1) 000360; DATA(1) 000041; BLANK COMMON(2) 000000

COMMON BLOCKS:

C003 CONSTS 000006
 C004 POINTS 000335
 C005 SPECS 012120
 C006 PISC 001264
 C007 TADR 000041

EXTERNAL REFERENCES (BLOCK, NAME)

C010 CPDS
 C011 ALUB
 C012 LAF
 C013 NCR34

STORAGE ASSIGNMENT (BLOCK, TYPE, RELATIVE LOCATION, NAME)

C001	000066	1356	0001	000251	2076	0001	00022	51L	0001	00050	55L	0001	000120	60L
C001	000165	81L	0001	000313	901L	0001	000321	903L	0005	00634	A	0006	000570	AM
C006	000624	AM	0006	000741	ANUM	0003	000000	ATM	0006	000004	ATOM	0006	000502	BU
C006	000521	EOP	0006	000036	CALCH	0000	R	000005	0005	000000	COEF	0007	000001	CONVG
C004	R	000032	CPH	0006	000625	CPRI	0006	R	000564	CPSUM	0006	000604	DATA	0005
C006	001167	UEAS	0000	R	000007	ULNT	0004	R	000064	ULVPT	0004	R	000047	DLVTP
C005	005360	ENLW	0006	001263	ENLSAV	0006	000000	ENN	0006	001261	ENNL	0006	000734	EN
C006	001073	ENTH	0006	000566	EQAT	0006	001112	FAZ	0006	001150	FOX	0004	R	001262
C004	R	000001	GLT	0007	L	000003	HP	0006	000572	HPP	0006	R	000101	GAMMAS
C004	R	005524	HO	0007	000030	IC	0007	000000	IOEBUG	0007	000015	IMAT	0004	R
C007	000015	INJPS	0007	000023	IONS	0007	000021	IP	0007	000037	IOSAVE	0007	000016	IOI
C007	000005	ISV	0007	000034	IT	0005	I	011444	IUSE	0000	I	000004	J	0007
C007	000025	JSOL	0007	I	000031	JSI	0007	000014	KMAT	0006	000463	LLMT	0007	000026
C007	000006	MOLES	0006	000626	NAME	0007	I	000024	NC	0007	000022	NEWB	0007	000040
C007	000012	NLM	0007	000017	NOF	0007	000020	NOMIT	0007	000007	NP	0007	I	000035
C007	000027	NRLAL	0007	I	000013	NS	0007	000000	NSPPI	0007	000010	NT	0007	000011
C006	00127	OXF	0004	000116	P	0003	000002	PATM	0006	001054	PECWT	0006	R	000565
C004	R	000117	PPP	0003	000003	PHAR	0003	000004	RHR	0006	000574	RH	0006	001206
C006	001207	MM	0006	R	000001	KNV	0006	001131	RTMP	0003	R	000005	RVR	0005
C007	000033	SHOCK	0005	011754	SLN	0004	000251	SONVEL	0007	L	000004	SP	0000	R
C004	R	000015	SSUM	0005	010770	SUB	0000	R	000003	SUMH	0006	000001	SUMS	0000
C006	R	000003	SO	0004	000150	T	0005	R	011610	TEMP	0006	000562	THIGH	0006
C006	R	000564	TLOW	0006	000557	TM	0006	000561	TMID	0004	R	000320	TORN	0007
C004	R	000001	TT	0004	R	000766	TTT	0004	000202	V	0004	R	000303	VLM
C007	L	000002	VOL	0007	000000	VPLS	0004	R	000234	WM	0006	000602	WP	0006

ORIGINAL PAGE IS
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00101 10 SUBROUTINE FROZEN
00101 20
00101 30 IFROZEN COMPOSITION EXPANSION ONLY)
00101 40
00101 50 COMMON /CONSTS/ ATMN,GMET,PATM,RBAR,RBR,RVR
00101 60 COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)
00101 70 1 GAMMAS(13),P(26),T(26),V(13),PP(13),WM(13),SONVEL(13),TTT(13)
00101 80 2 VLM(13),TOTN(13)
00101 90 3 COMMON/SPECIES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),HO(150)
00101 100 1 DELN(150),A(15,150),SUB(150,3),TUSE(150),TEMP(50,2),SLN(150)
00101 110 INCLUDE SPLCPK
00101 120 COMMON /MISC/ ENN,SUMN,TT,SU,ATOM(3,101),LLMT(15),BO(15),
00101 130 BOP(15,2),TM,LOW,THID,THIGH,PP,CPSUM,OF,EQRAT,
00101 140 HSURU,AM(2),HPP(2),PHI(2),VMIN(2),VPLS(2),MPI(2),
00101 150 DATA(16),AMI,CPRI,NAME(15,5),ANUM(15,5),PECM(15),
00101 160 ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15),RHOP,
00101 170 RMW(15),TLN,UXF(26),ENNL,ENSAVE,ENLSAV
00101 180 COMMON /INDX/ IDEBUG,CONVG,IP,HP,SP,ISV,MOLES,NP,NT,NPT,NLM,NS,
00101 190 KMAT,IMAT,IQI,NOF,NOMIT,IP,NEWIR,IONS,NC,JCOL,JLTO,
00101 200 NREAC,IC,JSI,VOL,SHOCK,IT,NFZ,CALCH,IQSAVE,LSAVE
00101 210
00101 220 LOGICAL CONVG,HP,SP,VOL
00101 230
00101 240 CONVG = .FALSE.
00101 250 TLN = ALOG(1)
00101 260 IF (VOL) RNV = RVR/(VLM(NPT)*WM(NFZ))
00101 270 51 SUMS=0.
00101 280 SUMH = 0.
00101 290 JSI = 1
00101 300 J = NPT
00101 310 NPT = NFZ
00101 320 CALL CPMS
00101 330 CC = CPSUM
00101 340 IF (.NOT.VOL) GO TO 55
00101 350 CC = CPSUM-1./WM(NFZ)
00101 360 PF = RNV*IT
00101 370 55 NPT = J
00101 380 DO 60 J = 1,NS
00101 390 IF (EN(J,NFZ)) .LE. 0.0) GO TO 60
00101 400 SS = S(J)
00101 410 IF (IUSE(J),EQ.0) SS=SS-ALOG(EN(J,NFZ))*PP*WM(NFZ)
00101 420 SUMS = SUMS+SS*EN(J,NFZ)
00101 430 IF (CONVG.OR.HP) SUMH=SUMH+HO(J)*EN(J,NFZ)
00101 440 60 CONTINUE
00101 450 IF (CONVG) GO TO 81
00101 460 IF (SP) DLNT=(SUMS-SU)/CC
00101 470 IF (HP) DLNT=(SUMH-HSUR0(1))/CC
00101 480 TLN=TLN-DLNT
00101 490 IF (ENL(1,0,5E-4) DLNT=-DLNT
00101 500 IF (ENL(1,0,5E-4) CONVG=.TRUE.
00101 510 IT = EXP(TLN)
00101 520 GO TO 11
00101 530 81 ITTEMP= IT
00101 540 SSUMN=TT*SUMS
00101 550 HSUMN=TT*SUMH
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GAMHAS(NPT) = CPSUM/(CPSUM-1./WM(NFZ))
VLM(NPT) = RVD*TT/(WM(NFZ)*PP)
WM(NPT) = WM(NFZ)
ULVPT(NPT) = -1.
OLVPT(NPT) = 1.
TOTN(NPT) = TOTN(NFZ)
PP(NPT) = PP
CPH(NPT) = CPSUM
IF (TT.LT.(TLOW-150.))GO TO 903
IF (INC -EQ. 0) RETURN
INC = 0
DO 901 J = 1,N5
IF (IUSE(J)).EQ. 0 .OR. IUSE(J).EQ. - 10000) GO TO 901
INC = INC+1
IF (LEN(J,NFZ) .LE. 0.0) GO TO 901
IF (TT.LT. TEMP(INC,1)-50. .OR. TT.GT. TEMP(INC,2)+50.) GO TO 903
901 CONTINUE
903 RETURN
NPT = NPT-1
RETURN
END

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FOR S LEWIS GAMEFF LEWIS GAMEFF
 N A 13 -10/25/79-17:38:33 (2)

SUBROUTINE GAMEFF ENTRY POINT 000176

STORAGE USED: CODE(1) 00017; DATA(1) 000044; BLANK COMMON(2) 000000

EXTERNAL REFERENCES (BLOCK, NAME)

0003 XPRN
 0004 SQRT
 0005 NERN34

STORAGE ASSIGNMENT (BLOCK, TYPE, RELATIVE LOCATION, NAME)

0001 000036 10L 0001 000025 1056 0001 000132 20L 0001 000152 50L 0000 R 000002 ANK
 0000 R 000000 CFA 0000 R 000005 CGAM 0000 R 000001 G 0000 R 000004 GM 0000 R 000003 GP
 0000 I 000000 I 0000 000014 INJPS

10 SUBROUTINE GAMEFF (V,GAMMAS,A,N,H)
 DIMENSION A(13),GAMMAS(13),H(13),V(13)
 DO 50 I = 2,N
 G = GAMMAS(I)
 ANK = +1.0
 IF (G -61. 1.0) GO TO 10
 G = 1.0010
 GP = G + 1.0
 CGAM = SQRT(G)*(2.0/GP)**(GP/(2.0*GM))
 CFA = CGAM*SQRT(2.0*G*(1.3 - (1.0/ALL))**((GM/G)))/GM
 IF (ABS(V(1)) - CFA) .LE. 5.0E-5) GO TO 53
 IF (G .LT. 2.0) GO TO 20
 IF (ANK .LT. 0.0) GO TO 50
 ANK = -1.0
 G = GAMMAS(I)
 GO TO 10
 20 G = G + ANK*(V(1) - CFA)
 IF (G -61. 1.0) GO TO 10
 IF (ANK .LT. 0.0) GO TO 50
 ANK = -1.0
 G = GAMMAS(I)
 GO TO 10
 50 H(1) = G
 RETURN
 END

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FOR S LEWIS-GAUSS-LEWIS-GAUSS
 11A 11-10/25/79-17:38:38 17.1

SUBROUTINE GAUSS ENTRY POINT 100411

STORAGE USED: C(011) 000431; DATA(0) 000126; BLANK COMMON(2) 000000

COMMON BLOCKS:

0003 DOUBLE 001500
 0004 INDEX 000041

EXTERNAL REFERENCES (BLOCK, NAME)

0001 NLEW34

STORAGE ASSIGNMENT (BLOCK, TYPE, RELATIVE LOCATION, NAME)

0001	000107 10L	0001	000011 110G	0001	000043 120G	0001	000062 127G	0001	000130 152G
0001	000161 167G	0001	000204 177G	0001	000115 18L	0001	000256 210G	0001	000257 213G
0001	000141 22L	0001	000361 23L	0001	000333 231G	0001	000167 31L	0001	000275 44L
0001	000303 47L	0001	000340 51L	0001	000020 8L	0001	000101 9L	0004	000036 CALCH
0000	000000 COLFX	0004	000001 CONVG	0003	000000 G	0004	000003 HP	0000	000056 I
0004	000030 IC	0004	000000 IOEBUG	0000	000071 INJPS	0004	000023 IONS	0004	000021 JP
0004	000037 IUSAVE	0004	000016 IQ1	0004	000005 ISV	0004	000034 IT	0004	000015 IUSE
0000	000054 IUSE1	0000	000057 J	0004	000026 JLIQ	0004	000025 JSOL	0004	000031 JSI
0001	000061 K	0004	000014 KMAT	0004	000040 LSAVL	0004	000006 MOLES	0004	000024 NC
0004	000022 ME-W	0004	000035 NF2	0004	000012 NLH	0000	000055 NN	0004	000017 NOF
0004	000020 NOMIT	0004	000007 NP	0004	000011 NPT	0004	000027 NREAC	0004	000013 NS
0004	000010 NT	0004	000033 SHOCK	0004	000004 SP	0000	000050 SUM	0000	000060 TEMP
0004	000002 TP	0004	000032 VOL	0003	0001510 X	0000	000052 Z		

00101	19	SUBROUTINE GAUSS	000000
00103	20	COMMON/DOUBLE/G(120,21),X(120)	000000
00104	30	COMMON /INDEX/ IOEBUG,CONVG,TP,HP,SP,ISV,MOLES,NP,NT,NPT,NLM,NS,	000000
00104	40	KMAT,IUSE,IQ1,NOF,NOMIT,JP,NEWB,IONS,NC,JSOL,JLIQ,	000000
00104	50	NREAC,IC,JSI,VOL,SHOCK,IT,NF2,CALCH,IOSAVE,LSAVE	000000
00105	60	COUPLE PRECISION COEFF(120),3,SUM,X,2	000000
00105	70	BEGIN ELIMINATION OF NTH VARIABLE	000000
00106	80	IUSE1=IUSE+1	000000
00107	90	DO 45 NP = 1,IUSE	000000
00107	100	IF (NP.NE.IUSE) GO TO 8	000002
00107	110	IF (G(N,N)) 31,23,31	000011
00107	120	SEARCH FOR MAXIMUM COEFFICIENT IN EACH ROW	000014
00107	130	DO 15 I=NP,IUSE	000014
00107	140	COEFF(I) = 1.0E36	000029
00107	150	IF (G(I,I).EQ.C.C.) GO TO 14	000047
00107	160	COEFF(I) = 0.	000051
00107	170	IF 16 CONTINUE	000054
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SUM = G(I,J)
IF (SUM.LT.0.) SUM=-SUM
IF (J.NE.NN) GO TO 9
Z = SUM
GO TO 10
9 IF (SUM.GT.COEFX(I)) COEFX(I)=SUM
10 CONTINUE
COEFX(I) = COEFX(I)/Z
18 CONTINUE
TEMP = 1.0E38
I=0
DO 22 J = NN,IUSE
IF (COEFX(J).GE. TEMP) GO TO 22
TEMP = COEFX(J)
I=J
22 CONTINUE
IF (I.EQ. 0) GO TO 23
INDEX I LOCATES EQUATION TO BE USED FOR ELIMINATING THE NTH
VARIABLE FROM THE REMAINING EQUATIONS
C INTERCHANGE EQUATIONS I AND NN
C IF (NN.EQ. 1) GO TO 31
DO 30 J = NN,IUSE1
Z=0(I,J)
G(I,J)=G(NN,J)
30 G(NN,J)=Z
DIVIDE NTH ROW BY NTH DIAGONAL ELEMENT AND ELIMINATE THE NTH
VARIABLE FROM THE REMAINING EQUATIONS
C
31 K = NN + 1
DO 36 J = K, IUSE1
IF (G(NN,NN).EQ.0.) GO TO 23
G(NN,J) = G(NN,J)/G(NN,NN)
36 IF (K.EQ. IUSE1) GO TO 45
DO 44 I = K,IUSE
DO 44 J = K,IUSE1
44 G(I,J) = G(I,J) - G(I,NN)*G(NN,J)
45 CONTINUE
BACKSOLVE FOR THE VARIABLES
C
47 J = K + 1
X(K) = 0.000
SUM = 0.0
IF (IUSE.LT. J) GO TO 51
DO 50 I = J,IUSE
50 SUM = SUM + G(I,I)*X(I)
51 X(K) = G(I,IUSE1) - SUM
K = K + 1
IF (K.NE. 0) GO TO 47
RETURN
23 IUSE = IUSE-1
RETURN
END

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HOW'S LEWIS-HCALC,LEWIS-HCALC
 0.0 0.0 -10/25/79-17:38:44 (9.0)

SUBROUTINE HCALC ENTRY POINT 000526

STORAGE USAGE: CODE(1) 000542; DATA(1) 000066; BLANK COMMON(2) 000000

COMMON BLOCKS:

CODE CONSTS 000006
 CODE POLCON 000010
 CODE POINTS 000101
 CODE SPICES 01.120
 CODE MISC 001264
 CODE INDX 000041
 CODE ECC 000003

EXTERNAL REFERENCES (BLOCK, NAME)

CODE CPYS
 CODE ALDB
 CODE FLOW
 CODE FLOW
 CODE NCR3

STORAGE ASSIGNMENT (BLOCK, TYPE, RELATIVE LOCATION, NAME)

CODE	000070	1436	0001	000107	15L	0001	000131	16L	0001	000145	1656	0001	000154	1726
CODE	000162	1776	0001	000204	2106	0001	000275	2276	0001	000170	30L	0001	000264	4L
CODE	000177	50L	0001	000432	500L	0001	000251	55L	0001	000265	56L	0001	000307	70L
CODE	000477	75L	0001	000010	76F	0001	000477	80L	0001	000024	85F	0001	000037	9L
CODE	000312	90L	0006	000034	A	0004	000001	AG	0007	000570	AM	0007	000624	AM1
CODE	000000	AM2	0007	000741	ANUM	0003	000000	ATM	0007	000004	ATOM	0004	000004	HLK
CODE	000502	40	0007	000521	BOP	0010	000036	CALCH	0006	000000	COEF	0010	000001	COMV6
CODE	000032	CFM	0007	000625	CFM1	0007	000564	CPSUM	0007	000604	DATA	0006	000670	DELN
CODE	000002	CFM2	0007	000167	DEMS	0005	000064	ULVPT	0005	000047	ULVTP	0006	000734	EN
CODE	000000	END	0000	000007	ENJ	0006	000360	ENLN	0007	001263	ENLSAV	0007	000000	ENN
CODE	000161	ENML	0007	000162	ENSAVE	0007	001073	ENTH	0007	000566	EQWAT	0007	001112	FAZ
CODE	000150	FOR	0003	000001	GHEI	0011	000000	GRAPH	0010	000003	HP	0007	000572	HPP
CODE	000067	HSPUR	0005	000000	HSUM	0006	000524	HO	0000	000005	I	0010	000030	IC
CODE	000000	IDLBUB	0004	000002	IL	0010	000015	IMAT	0000	000004	INJPS	0010	000023	IONS
CODE	000021	IP	0010	000037	ICSAVE	0010	000016	LOI	0000	000006	IS	0010	000005	ISV
CODE	000034	IT	0006	001444	LOSL	0004	000003	ITERO	0010	000031	J	0010	000026	JL10
CODE	000001	JOUT	0010	000025	J5OL	0000	000004	K	0010	000014	KMAT	0010	000012	L
CODE	000043	LLMT	0010	000040	LSAVE	0004	000005	MOL	0010	000006	MOLES	0000	000003	N
CODE	000026	MMH	0010	000024	MC	0010	000022	NEAR	0010	000035	NFZ	0010	000017	NDF
CODE	000000	NOM11	0010	000007	NP	0010	000011	NPT	0010	000027	NREAL	0010	000013	NS
CODE	000000	NSPFI	0010	000010	NT	0007	000741	NUM	0007	000565	OF	0004	000006	OK
CODE	001277	OFF	0003	000002	FATH	0007	001054	PFCWT	0007	000563	PF	0003	000003	RRAR
CODE	000000	RRR	0007	000574	RH	0007	001206	RHOP	0007	001207	RHM	0010	001131	RTLMF
CODE	000000	RRR	0010	000570	S	0010	000033	SHOCK	0006	001174	SL4	0010	000004	SP
CODE	000000	SSM	0006	001170	SMB	0007	000001	SUMN	0007	000003	50	0006	0011610	TEMP

0007	000561	IM10
0010	000032	VOL

0007 R 000557 IM
0007 000576 VMIN

0007	R	000560	FLOW
0007	R	000002	IT
0004		000007	ZERO

0007 P 001226 ILN
0000 P 000001 TSAVE
0007 P 000602 LP

DATE	TIME	LOCATION	WIND DIRECTION	WIND SPEED	SEA STATE	TEMPERATURE	HUMIDITY	PRESSURE	REMARKS
01-07-68	0800	OFF SHORE	090	10 KTS	3	28.5	75%	1010	GOOD VISIBILITY
01-07-68	1200	OFF SHORE	090	12 KTS	3	28.5	75%	1010	GOOD VISIBILITY
01-07-68	1600	OFF SHORE	090	10 KTS	3	28.5	75%	1010	GOOD VISIBILITY

```

SUBROUTINE HCALC
C CALCULATE ENTHALPY FOR PROPELLANT USING COEFFICIENTS
COMMON /CONSTS/ ATMN,GHE1,PAIM,RBAR,RBR,RVR
COMMON /HOLCON/ END,AG,IE,I2EPO,BLK,MOL,OX,ZERO
COMMON /PJNITS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)
COMMON /SPECS/COLF(2,7,150),S(150),EM(150,13),ENLN(150),HO(150)
C 1,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2),SLN(150)
INCLUDE SPECPH
COMMON /MISC/ LNN,SUMN,TT,S0,ATOM(3,101),LLM(151),BO(15),
1 HOP(15,2),TM,TLOW,TMIO,THIGH,PP,CPSUM,OF,EQRAT,
2 HSUBU,AM(2),HPP(2),RH(2),VMIN(2),VPLS(2),WP(2),
3 DATA(16),AMI,CPR1,NAME(15,5),ANUM(15,5),PECWT(15),
4 ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15),RHOP,
5 RMW(15),ALN,OXF(26),ENML,ENSAVE,ENLSAV
COMMON /INDX/ IDBUG,CONVG,TP,MP,SP,ISV,MOLES,NP,NT,NPT,L,NS,
1 WHAT,IMAT,IQL,NOF,NOMIT,IP,NEWN,IONS,NC,JSOL,JLIQ,
2 NREAC,IC,J,VOL,SHOCK,IT,MFZ,CALCH,IOSAVE,LSAVE
COMMON /CCC/ GRAPH,JOUT,DEMAND
C
C DIMENSION NUM(15,5)
EQUIVALENCE (ANUM,NUM)
INTEGER AG,BLK,FAZ,FOX,OX
LOGICAL CALCH,MOLES,SHOCK,VOL
TSAVE = TT
IF (AM(1).GT. 0.0 .AND. AM(2).GT. 0.0) GO TO 4
AM1 = AM(2)
IF (AM(2).LE. 0.0) AM1 = AM(1)
GO TO 9
4 AM1=(0.5+1.)*AM(1)+AM(2)/(AM(1)+OF*AM(2))
9 TM = 0.
IF (PE,GT.0.) TM = ALOG(P/PE*AM1)
SSUM(NPT) = 0.
HPP(1) = 0.
HPP(2) = 0.
HSUBU = 0.
CPH1 = 0.
AN = (1.+OF)
LOOP ON REACTANTS. IF OXIDANT, K = 1, IF FUEL, K = 2.
DO J=0,N-1,NREAC
K=2
IF (FOX(N),EQ.OXIDANT)
IF (NAME(N,5),NE.I2EPO) GO TO 90
IF (.NOT.CALCH) GO TO 15
IT = REENF(N)
10 IT = T/TA - 1
15 IF (SHOCK) GO TO 16
IF (IT -LT. TLOW - 100.0 .OR. IT .GT. THIGH + 1000.0) GO TO 75
16 IF (TLOW)

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C-29

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+0 FOR

```

IF (J-NE-0) GO TO 90
DO 10 J=1,L
10 DATA(J) = 0.0
DO 30 I = 1,N
IF (ANUMIN,I) .LL. 0.0) GO TO 50
DO 20 J=1,L
20 IF (LLHT(J) .EQ. NAME(N,I)) GO TO 30
30 DATA(J) = DATA(J) + ANUMIN,I)
50 IS=0
DO 70 J=1,NS
IF (IUSL(J).EQ.0)GO TO 55
IS = IS+1
IF (FAZIN).EQ.0)GO TO 70
IF (IT-6T-TEMP(15,2).AND-TEMP(15,2).NE-THIGH) GO TO 70
IF (IT-6T-TEMP(15,1).AND-TEMP(15,1).NE-TLOW) GO TO 70
70 CONTINUE
55 IF (FAZIN).NE.0)AND-FAZIN.NE.BLK) GO TO 70
56 DO 60 I=1,L
60 IF (I+1,J) .NE. DATA(I)) GO TO 70
NUMIN(I) = J
GO TO 90
70 CONTINUE
80 DO 80 I=1,L
90 IF (I-MOLE) ENJ = PECWTIN/MP(K)
IF (I-MOLE) ENJ = PECWTIN/RMIN(I)
ENJ = ENJ/ANN
IF (I-EU-1) ENJ = ENJ*OF
IF (NAME(N,5).NE-12ER0)GO TO 500
I = NS
NS = J
TLN = ALOG(TT)
IF (I-MOT-CALCH) ENJ,NPT) = ENJ
CALL CPHS
NS = 1
IF (H(I,J).GT.-.01 .AND. H(I,J).LT..01) H(I,J) = 0.
RTLN(I) = TT
IF (V(I) H(I,J)-H(I,J)-1.
ENTH(I) = RPAROT(H(I,J)
CPR1 = CPR1 + CPSUM
500 HSUB = HSUB + ENTH(I)*ENJ
HPPIN = HPPIN + ENTH(I)*ENJ
900 SSUM(NPT) = SSUM(NPT) + ENJ*(S(I,J) - ALOG(ENJ) - TM)
TT = TAVE
HSUB = HSUB/RPAR
RETURN
75 RTLNOUT,76)
76 FORMAT (//20X,5TH REACTANT TEMPERATURE OUT OF RANGE OF THERMO DATA
11X, H(CALC/))
RETURN
8J -RTLNOUT,85) N
85 FORMAT (//20X,12,4TH REACTANT IS NOT IN THERMO DATA IN H(CALC/))
RETURN
END

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C-32

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FORM 5, 11-15-MAIN-11-15-MAIN
10-1 (3-10/25/79-17:38:58 (17,1)

MAIN PROGRAM

STORAGE USED: C000(1) 001235; DATA(1) 000424; BLANK COMMON(2) 000000

COMMON BLOCKS:

C0005 CONSTS 000000
C0009 MLCOR 000010
C0015 POINTS 000335
C0016 SPECS 012120
C0017 MISC 001264
C0018 INDX 000041
C0019 PLNF 000106
C0020 CCC 000003

EXTERNAL REFERENCES (BLOCK, NAME)

C0013 RUYES
C0014 MFSIM
C0015 PAGIT
C0016 CHRST
C0017 GOUT
C0018 HUATAI
C0019 PLACT
C0020 LCPHS
C0021 RUCOR
C0022 RUCOR
C0023 SLACH
C0024 THERM
C0025 DELON
C0026 ROCKE
C0027 SHOR
C0028 MFSIM
C0029 NINTP
C0030 NINTP
C0031 NINTP
C0032 NINTP
C0033 NINTP
C0034 NINTP
C0035 NINTP
C0036 NINTP
C0037 NINTP
C0038 NINTP
C0039 NINTP
C0040 NINTP
C0041 NINTP
C0042 NINTP
C0043 NINTP
C0044 NINTP
C0045 NINTP
C0046 NINTP

STORAGE ASSIGNMENT (BLOCK, TYPE, RELATIVE LOCATION, NAME)

BLOCK	TYPE	RELATIVE LOCATION	NAME
C0001	000000	100	000000
C0002	000000	100	000000
C0003	000000	100	000000
C0004	000000	100	000000
C0005	000000	100	000000
C0006	000000	100	000000
C0007	000000	100	000000
C0008	000000	100	000000
C0009	000000	100	000000
C0010	000000	100	000000
C0011	000000	100	000000
C0012	000000	100	000000
C0013	000000	100	000000
C0014	000000	100	000000
C0015	000000	100	000000
C0016	000000	100	000000
C0017	000000	100	000000
C0018	000000	100	000000
C0019	000000	100	000000
C0020	000000	100	000000
C0021	000000	100	000000
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C0028	000000	100	000000
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C0031	000000	100	000000
C0032	000000	100	000000
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C0034	000000	100	000000
C0035	000000	100	000000
C0036	000000	100	000000
C0037	000000	100	000000
C0038	000000	100	000000
C0039	000000	100	000000
C0040	000000	100	000000
C0041	000000	100	000000
C0042	000000	100	000000
C0043	000000	100	000000
C0044	000000	100	000000
C0045	000000	100	000000
C0046	000000	100	000000


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00111 140
00111 150
00111 160
00112 170
00112 180
00112 190
00113 200
00113 210
00113 220
00114 230
00115 240
00116 250
00124 260
00126 270
00127 280
00130 290
00130 300
00130 310
00131 320
00131 330
00132 340
00132 350
00133 360
00133 370
00133 380
00134 390
00135 400
00136 410
00140 420
00143 430
00144 440
00145 450
00146 460
00150 470
00151 480
00152 490
00153 500
00154 510
00155 520
00156 530
00157 540
00160 550
00161 560
00162 570
00163 580
00164 590
00165 600
00166 610
00167 620
00170 630
00171 640
00173 650
00173 660
00174 670
00175 680
00176 690

3
DATA116),AMT,CPR1,NAME115,5),ANUM115,5),PECWT115),
LNTH115),FAZ115),RTMP115),FOX115),DENS115),RHOP,
EMW115),ILW,ORF(26),ENNL,ENSAVE,ENLSAV
COMMON /INDX/ IDBUG,CONVG,TP,MP,SP,ISV,MOLES,MP,NT,NPT,L,MS,
KMAT,IMAT,IGI,NOF,MOMIT,IP,NEWR,IONS,NC,J5OL,JLTO,
NREAC,IC,J5I,VOL,SHOCK,II,NFZ,CALCH,IQSAVE,LSAVE
COMMON /PERF/ PCPT26),VMOC113),SPIM113),VACT113),SUBAR113),
SUPAR113),APP113),AEAT113),EQL
COMMON /CELL/ GRAPH,JOUT,DEMAND
INTEGER BLANK,DATA,END,INSERT,OMIT,REAC,SUB,YHRM
DATA INSERT,MIT,NMLT,REAC,THRM/WHINSE,WHUMIT,WHNAME,WHREAC,WHYHRM/
DATA MLOW/MHLOW /
DIMENSION INSERT(15),NCD(41),OMIT(3,2)
EQUIVALENCE (IDLN,INSERT),IENLN,OMIT),IMIX,ORF),IOF,ORF),ISO,SOI
LOGICAL CALCH,UEIN,EQL,ERATIO,FA,FPCT,MP,IONS,MMHG,MOLES,NEWR,
NSUM,OF,PSIA,RKT,SHOCK,SP,SV,TP,TV,UV,VOL
1
LOGICAL RUYES,FIRST
REAL MIX(26)
NAMELIST /INPT2/ ULIN,ERATIO,FA,FPCT,MP,IDBUG,IONS,MIX,MMHG,NSUM,
OF,P,PSIA,RKT,SO,SHOCK,SO,SP,SV,T,TP,TV,UV,V
1
FIRST=.TRUE.
CALL MPSTINT
1 WRITE(JOUT,400)
DO 300 I=1,26
MIX(I) = 0.0
P1112 = 0.
T1112 = 0.
V1112 = 0.0
IF = .FALSE.
HF = .FALSE.
TV = .FALSE.
UV = .FALSE.
SV = .FALSE.
MRT = .TRUE.
SHOCK = .FALSE.
DEIN = .FALSE.
MMHG = .FALSE.
PSIA = .TRUE.
NSUM = .FALSE.
IONS = .FALSE.
IDBUG = 0
FA = .FALSE.
OF = .TRUE.
ERATIO = .FALSE.
FPCT = .FALSE.
EQL = .TRUE.
MLOW = .FALSE.
MLOW = .FALSE.
CALL FOUT11
JOUT26
JOUT26
IF = 0.0,CTYBL YES FOR PRINT TO PRINT FILE',IS1) JOUT26

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00000 700 000064
00001 710 000065
00002 720 000065
00003 730 000070
00004 740 000074
00005 750 000100
00006 760 000104
00007 770 000110
00008 780 000114
00009 790 000120
00010 800 070124
00011 810 000130
00012 820 000134
00013 830 000140
00014 840 000144
00015 850 000145
00016 860 000150
00017 870 000155
00018 880 000157
00019 890 000175
00020 900 000175
00021 910 000175
00022 920 000211
00023 930 000211
00024 940 000212
00025 950 000213
00026 960 000216
00027 970 000225
00028 980 000225
00029 990 000233
00030 1000 000233
00031 1010 000241
00032 1020 000241
00033 1030 000241
00034 1040 000243
00035 1050 000244
00036 1060 000244
00037 1070 000244
00038 1080 000246
00039 1090 000247
00040 1100 000252
00041 1110 000256
00042 1120 000266
00043 1130 000266
00044 1140 000277
00045 1150 000310
00046 1160 000310
00047 1170 000315
00048 1180 000325
00049 1190 000330
00050 1200 000330
00051 1210 000354
00052 1220 000354
00053 1230 000367
00054 1240 000367
00055 1250 000367

203
CONTINUE
CALL PAGIT
CALL CHR$12(1)
CALL GOUTI*LE=15 CHEMICAL EQUILIBRIUM PROGRAM*,34)
CALL GOUTI* ,1)
CALL GOUTI* ,1)
CALL GOUTI* ,1)
CALL GOUTI* ,1)
CALL GOUTI* 1 - READ THERMODYNAMIC DATA FROM CARDS*,39)
CALL GOUTI* 2 - READ LOW TEMP EXTENSION THERMO DATA*,40)
CALL GOUTI* 3 - SELECT REACTANTS*,21)
CALL GOUTI* 4 - OMIT SPECIES FROM THERMO DATA*,34)
CALL GOUTI* 5 - INSERT CONDENSED SPECIES*,29)
CALL GOUTI* 6 - BEGIN NAMELIST INPUT*,25)
CALL GOUTI* RETURN - TERMINATE PROGRAM*,27)
ICARD=0
CALL CHR$12(4)
CALL ROTAT(1,ICARD,5203)
IF (ICARD.EQ.0) GO TO 3
IF (ICARD.LT.1 .OR. ICARD.GT.6) GO TO 203
GO TO 190,39,11,205,108,210),ICARD
C
CALL SUBROUTINE TO READ REACTANT CARDS
C
11 NSEIT = 0
NOMIT = 0
MOLES = .FALSE.
CALL REACT(1FIRST)
IF (LE.EQ.0) WRITE(JOUT,52)
52 FORMAT(12H)ERROR IN REACTANT CARDS)
CALCH = .FALSE.
DO 755 I = 1,NREAC
755 IF (NAME(I,5) .EQ. 12) CALCH = .TRUE.
GO TO 203
C
READ LOW TEMPERATURE EXTENSION THERMO DATA
39 CALL LTCPHS
GO TO 203
C
READ THERMO DATA FROM CARDS AND STORE ON TAPE "
90 NEW = .TRUE.
REWINO "
CALL GOUTI*ADD THERMO DATA HERE*,20)
READ(5,5) TLOW,TMID,THIGH
5 FORMAT (3F10.3)
WRITE (4,5) TLOW,TMID,THIGH
97 READ (5,10) DATA,NCD(1)
10 FORMAT(34H,6X,2A3.4(A2,F3.0),A1.2F10.3,11S)
IF (DATA(1).EQ.0) DATA(1)=END
WRITE (4,10) DATA
IF (DATA(1).EQ.0) GO TO 203
READ (5,20) (DATA(I), I = 1,5),NCD(2), (DATA(J), J = 6,10),NCD(3),
1 (DATA(I), I = 1,14),NCD(4)
20 FORMAT(5L15.8,15/5L15.8,15/4L15.8,120)
WRITE (4,21) (DATA(I), I = 1,14)
21 FORMAT(5L15.8/5L15.8/4L15.8)
DO 25 I = 1,4
3 IF (NCD(I).EQ.1) GO TO 25

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4/23/70

MAIN0041

MAIN0053


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003372 000372
003404 000404
000404 000404
000404 000404
000404 000404
000406 000406
000406 000406
000407 000407
000414 000414
000421 000421
000424 000424
000437 000437
000437 000437
000437 000437
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000511 000511
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000553 000553
000553 000553
000561 000561
000566 000566
000571 000571
000576 000576
000577 000577
000601 000601
000603 000603
000607 000607

WRITE(JOUT,22) (DATA(I),J=1,3)
22 FORMAT(28HORDERP IN ORDER OF CARDS FOR ,34H)
25 CONTINUE
GO TO 97

C CHECK INSERT CARDS
104 CONTINUE
CALL PAGIT
CALL GOUTI*TYPE SPECIES TO INSERT(I PER LINE)*,34H)
CONTINUE
181 CALL RUCHEP(RUOM,2,-1,8203)
INSERT=INSERT+1
DECODE(207,RUOM) (INSERT(I,INSERT), 1,1,1)
GO TO 181

C CHECK UNIT CARDS
205 CONTINUE
CALL PAGIT
CALL GOUTI*TYPE SPECIES TO OMIT FROM THERMO DATA*,37H)
CONTINUE
206 CALL RUCHEP(RUOM,2,-1,8208)
NOMIT=NOMIT+1
DECODE(207,RUOM) (NOMIT(I,NOMIT), 1,1,1)
FORMAT(34H)
GO TO 206

208 CONTINUE
NEWRE=.TRUE.
REWINO 4
GO TO 203

C BEGIN NAMELIST INPT2
210 RHOF = 0.0
SO = 0.0
SPE=.FALSE.
VCL = .FALSE.
VT = 1
CALL PAGIT
IF(POYESI*TYPE YES FOR PRESENT INPT2 NAMELIST*,35H)
1 RITE(6,INPT2)
RITE(6,211)
FORMAT(* BEGIN NAMELIST INPT2 INPUT*)
HEADS,INPT2)
CALL PAGIT
RITE(JOUT,INPT2)
IF(.NOT.TV.AND..NOT.UV.AND..NOT.SV) GO TO 304
VOL = .TRUE.
DO 1304 I=1,26
IF (P(I)) .GT. 0.0) P(I) = 1.0/P(I)
IF (V(I)) .GT. 0.0) P(I) = V(I)
IF (P(I)) .LE. 0.0) GO TO 1305
1304 IF = 1
1305 IF = TV
IF = UV
IF = SV
GO TO 304
304 DO 305 I=1,26

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1820 IF (F(1)) .LE. 0.01 GO TO 322
1830 NP = 1
1840 IF (MMHG) P(NP) = P(NP)/760.
1850 IF (PSIA) P(NP) = P(NP)/PATM
1860 IF (NSQM) P(NP) = P(NP)/ATM
1870 305 IF (NSQM) P(NP) = P(NP)/ATM
1880 322 00 307 11 = 1.26
1890 IF (T(1)) .LE. 0.01 GO TO 722
1900 NT = 11
1910 722 00 625 151 = 1.26
1920 IF (MIX(151)) .GT. 0.01 GO TO 323
1930 724 FORMAT (7/45X,40HNO INPT2 VALUE GIVEN FOR FA, FPCT, OR OF//)
1940 724 IF (M(12)) .GT. 0.01 OXFL = MP(11)/MP(12)
1950 30 10 333
1960 323 OXFL = MIX(151)
1970 IF (FA) OXFL = 1./ MIX(151)
1980 IF (FPC1) OXFL = (100.- MIX(151))/ MIX(151)
1990 IF (NOT-ERRATION) GO TO 333
2000 EQRT = MIX(151)
2010 IF (EQRT-0.1) EQRT = 1.000005
2020 OXFL = 1-EQRT*VMIN(2)-VPLS(21)/(VPLS(11)+EQRT*VMIN(11))
2030 333 OXFL(151) = OXFL
2040 625 NOF = 151
2050 745 IF (NOT-IONS .OR. LLMTIL) .EQ. IE) GO TO 746
2060 L = L+1
2070 IF (LLMTIL) .NE. IE) NEWR=.TRUE.
2080 REWIND 4
2090 LLMTIL = IE
2100 BOPIL(1) = 0.
2110 BOPIL(2) = 0.
2120 60 10 748
2130 746 IF (LLMTIL) .NE. IE) GO TO 748
2140 00 747 J=1,NS
2150 747 IF (AL(J)) .NE. 0.01 IUSE(J) = - 10000
2160 L = L-1
2170 748 IF (NEWR) CALL SEARCH
2180 INITIAL ESTIMATES
2190 SO = SU/REAR
2200 LNN = .1
2210 ENNL = -2.3025851
2220 SUMN = ENN
2230 00 432 J=1,NS
2240 IF (IUSE(J)) .GT. 0 IUSE(J) = -IUSE(J)
2250 IF (IUSE(J)) .EQ. -10000 .AND. IONS) IUSE(J) = 0
2260 ENL(J) = 0.
2270 ENL(J) = 0.
2280 IF (IUSE(J)) .NE. 0 GO TO 432
2290 ENL(J) = ENN/INS - NC)
2300 ENL(J) = ALUG(ENL(J))
2310 432 CONTINUE
2320 ICL = L+1
2330 IF (MC.EQ.0) .OR. INSERT.EQ.0) GO TO 790
2340 00 302 1=1,NS
2350 00 301 J=1,NS
2360 IF (IUSE(J)) .EQ. 0 GO TO 301
2370

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MAIN0090

MAIN0141
MAIN0145

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MAIN0152

MAIN0153

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00 299 IST = 1,3
299 IF (SUB(J,IST) .NE. ENSEBT(IST,1)) GO TO 301
    IQ1 = 1,1
    IUSE(J) = -IUSE(J)
    GO TO 302
301 CONTINUE
302 CONTINUE
790 IF (I-NOT, TP .AND., .NOT, HP .AND., .NOT, SP) GO TO 791
    CALL THERMP
    GO TO 800
791 IF (I-ETN) CALL UETON
    IF (IRKT) CALL RUCKET
    IF (SHOCK) CALL SHCK
    800 NSERT = 0
    GO TO 1
3    CONTINUE
    CALL MPSTRM
    STOP
END

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2560

END FOR

SUBROUTINE MATRIX ENTRY POINT U01063

STORAGE USED: C00E111 U01107; DATA(0) U00116; BLANK COMMON(2) 000000

COMMON BLOCKS:

0001 POINTS 000335
 0004 SPECLS 012120
 0005 RISC 001264
 0006 DOUBLE 001560
 0007 160X 000041

INTERNAL REFERENCES (BLOCK, NAME)

0010 NLRYS

STORAGE ASSIGNMENT (BLOCK, TYPE, RELATIVE LOCATION, NAME)

0001	000102	1246	0001	000103	1276	0001	000126	1406	0001	000215	1546	0001	000244	1616
0001	000672	175L	0001	000677	185L	0001	000453	2176	0001	001011	230L	0001	000567	2446
0001	000606	2476	0001	000623	2576	0001	001026	260L	0001	000757	3036	0001	001023	3176
0001	000276	55L	0001	000346	59L	0001	000372	62L	0001	000376	64L	0001	000511	65L
0001	000405	70L	0004	R 000034	A	0005	000570	AM	0005	000624	AM	0004	000741	AMUM
0005	R 000004	ATUM	0005	R 000502	80	0005	000521	80P	0007	000036	CALCH	0004	000000	COEF
0007	L 000001	CONVG	0003	000032	CPR	0005	000625	CPR1	0005	R 000564	CPSUM	0005	000004	DATA
0004	000576	DELN	0005	001167	DENS	0003	000064	DLVPT	0003	000047	DLVTP	0004	R 002734	EN
0004	R 000013	ENR6Y	0004	R 0005360	ENLN	0005	001263	ENLSAV	0005	R 000000	ENN	0005	001261	ENNL
0005	001262	ENSAVE	0005	001073	ENTH	0005	000566	EQAT	0000	R 000010	F	0005	001112	FAZ
0005	001150	FOX	0006	D 000000	G	0003	000101	GAMMAS	0007	L 000003	HP	0005	000572	HPP
0005	R 000567	HSUBU	0003	R 000000	HSUM	0004	R 005524	HQ	0000	I 000003	I	0007	000030	IC
0007	000000	IDLRUG	0007	I 000015	IMAT	0000	000023	INJPS	0007	000002	IQ3	0007	000021	IP
0007	000037	IQSAVE	0007	I 000016	IQ1	0000	I 000001	IQ2	0000	I 000002	IQ3	0007	000005	ISV
0007	000034	IT	0004	I 011444	IUSE	0000	I 000007	J	0007	000026	JLIQ	0007	000025	J50L
0007	000031	J51	0000	I 000004	K	0000	I 000006	KK	0007	I 000014	KMAT	0007	I 000012	L
0005	000063	LLMT	0007	000040	LSAVE	0007	000006	MOLES	0005	000626	NAME	0007	000024	MC
0007	000002	MEWR	0007	000035	NF2	0007	000017	NOF	0007	000020	NOMIE	0007	000007	NP
0007	I 000011	OPT	0007	000027	MRAC	0007	I 000013	NS	0000	I 000000	NSPPI	0007	000010	NT
0005	000565	OF	0005	001227	OXF	0003	000116	P	0005	001054	PECMI	0005	000563	PP
0005	000217	PPF	0005	000574	PH	0005	001206	RHOP	0005	001207	RHM	0005	001131	STEMP
0004	R 002576	S	0007	000033	SHOCK	0004	011754	SLN	0003	000251	SONVLL	0007	L 000004	SP
0000	R 000011	SS	0000	F 000005	SSS	0004	000015	SSUM	0004	010770	SUB	0005	R 000001	SUMM
0005	R 000003	SD	0003	000150	T	0004	011610	TEMP	0000	R 000012	TERMI	0005	000562	THIGH
0005	001226	TLN	0005	000560	TLOW	0005	R 000557	TM	0005	000561	THIO	0003	000320	TOTM
0007	L 000002	TP	0005	R 000002	TT	0003	000266	TTT	0003	000202	V	0003	000303	VLM
0005	000576	VMIN	0007	L 000032	VOL	0005	000600	VPLS	0003	000234	WM	0005	000602	WP
0005	D 001310	A												

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1001 SUBROUTINE MATRIX
1002
1003 COMMON/POINTS/MSUM(13),SSUM(13),CPR(13),ULVPT(13),ULVPT(13)
1004 1 ,GAMMA(13),P(26),T(26),V(13),PPP(13),MM(13),SONVEL(13),TTTT(13)
1005 2 ,VLM(13),TOTM(13)
1006 COMMON/SPICES/COEF(2,7,150),S(150),EM(150,13),ENL(150),H(150)
1007 1 ,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2),SLN(150)
1008 INCLUDE SPECPH
1009 COMMON /MISC/ ENN,SUMN,TT,SD,ATOM(13,10),LLMT(15),BD(15),
1010 /MISC/ BOP(15,2),TH,TLOW,IMID,THIGH,PP,CPSUM,GF,EQRAT,
1011 /MISC/ HSUBU,AMU(2),HPP(2),RH(2),VMIN(2),VPLS(2),WP(2),
1012 /MISC/ DATA(16),AMI,CPRI,NAME(15,5),ANUM(15,5),PECWT(15),
1013 /MISC/ ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15),RHOP,
1014 /MISC/ RM(15),TLN,OXF(26),ENNL,ENSAVE,ENLSAV
1015 COMMON /DOUBLE/ G(20,21), X(20)
1016 COMMON /INUX/ IDEBUG,CONVG,TP,HP,SP,ISV,MOLES,NP,NT,NPT,L,NS,
1017 /INUX/ KMAT,IMAT,IQ1,NOF,NOMIT,IP,NELWR,IONS,NC,JSOL,JLJO,
1018 /INUX/ NPEAC,IC,JSI,VOL,SHOCK,IT,NFZ,CALCH,IQSAVE,LSAVE
1019
1020 DOUBLE PRECISION G,X
1021 LOGICAL CONVG,HP,SP,TP,VOL
1022
1023 IQ2 = IQ1 + 1
1024 IQ3 = IQ2 + 1
1025 KMAT = IQ3
1026 IF (.NOT. CONVG. AND. .IF) KMAT = IQ2
1027 IMAT = KMAT - 1
1028 CLEAR MATRIX STORAGES TO ZERO
1029 DO 211 I=1,IMAT
1030 DO 211 M=1,KMAT
1031 G(I,M) = 0.003
1032 SSS = 0.
1033 HSUM(NPT) = 0.
1034 BEGIN SET UP OF ITERATION MATRIX
1035 MK = L
1036 DO 65 J=1,NS
1037 IF (IUSE(J).LT.0) GO TO 65
1038 IF (IUSE(J).GT.0) GO TO 70
1039 F = (H(J)-S(J)+ENLN(J)*TH)*EN(J,NPT)
1040 SS = H(J)*EN(J,NPT) - F
1041 TERM1 = H(J)*EN(J,NPT)
1042 IF (KMAT .EQ. 102) TERM1 = F
1043 DO 55 I = 1, L
1044 CALCULATE THE ELEMENTS R(I,M)
1045 IF (ALL(J) .EQ. 0.) GO TO 55
1046 DO 15 M=1, L
1047 G(I,M) = G(I,M) + A(M,J)*A(I,J)*EN(J,NPT)
1048 G(I,IQ1) = G(I,IQ1) + ALL(J)*EN(J,NPT)
1049 G(I,IQ2) = G(I,IQ2) + A(I,J)*TERM1
1050 IF (CONVG .OR. TP) GO TO 55
1051 G(I,IQ3) = G(I,IQ3) + ALL(J)*F
1052 IF (SPI G(IQ2,I) = G(IQ2,I) + ALL(J)*SS
1053 55 CONTINUE
1054 IF (KMAT .EQ. 102) GO TO 64
1055 IF (CONVG .OR. HP) GO TO 59

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00202      G(IQ2,IQ1) = G(IQ2,IQ1) + SS
00203      G(IQ2,IQ2) = G(IQ2,IQ2) + H0(J)*SS
00204      G(IQ2,IQ3) = G(IQ2,IQ3) + IS(J) - ENLN(J)*TM)*F
00205      GO TO 62
00206      59 G(IQ2,IQ2) = G(IQ2,IQ2) + H0(J)*2*EN(J,NPT)
00207      IF (CONVG) GO TO 64
00208      G(IQ2,IQ3) = G(IQ2,IQ3) + H0(J)*F
00209      62 G(IQ1,IQ3) = G(IQ1,IQ3) + F
00210      64 G(IQ1,IQ2) = G(IQ1,IQ2) + TERM1
00211      GO TO 65
00212      C CONDENSED SPECIES
00213      70 KK = KK + 1
00214      DO 75 I = 1,L
00215      G(I,KK) = A(I,J)
00216      75 G(I,KMAT) = G(I,KMAT) - A(I,J)*EN(J,NPT)
00217      G(KK,IQ2) = H0(J)
00218      G(KK,KMAT) = H0(J) - S(IJ)
00219      HSUM(NPT) = HSUM(NPT) + H0(J)*EN(J,NPT)
00220      IF (.NOT. SP) GO TO 65
00221      SSS = SSS + S(IJ)*EN(J,NPT)
00222      G(IQ2,KK) = S(IJ)
00223      65 CONTINUE
00224      SSS = SSS + G(IQ2,IQ1)
00225      HSUM(NPT) = HSUM(NPT) + G(IQ1,IQ2)
00226      G(IQ1,IQ1) = SUMN - ENN
00227      REFLECT SYMMETRIC PORTIONS OF THE MATRIX
00228      K = IQ1
00229      IF (HP .OR. CONVG) K = IQ2
00230      DO 102 I = 1,K
00231      DO 102 J = 1,K
00232      G(I,J) = G(I,J)
00233      102 COMPLETE THE RIGHT HAND SIDE
00234      IF (CONVG) GO TO 175
00235      145 I=1,L
00236      A(I) = B(I) - G(I,IQ1)
00237      G(I,KMAT) = G(I,KMAT) + X(I)
00238      G(IQ1,KMAT) = G(IQ1,KMAT) + ENN*SUMN
00239      COMPLETE ENERGY ROW AND TEMPERATURE COLUMN
00240      IF (KMAT .EQ. IQ2) GO TO 185
00241      IF (SP) ENRGY = 50*ENN*SUMN - SSS
00242      IF (HP) ENRGY = HSUM(NPT)
00243      G(IQ2,IQ3) = G(IQ2,IQ3) + ENRGY
00244      175 G(IQ2,IQ2) = G(IQ2,IQ2) + CPSUM
00245      185 IF (.NOT. VOL .OR. CONVG) RETURN
00246      C CONSTANT VOLUME MATRIX
00247      K = IC1 - 1
00248      IF (KMAT .EQ. IQ2) GO TO 230
00249      DO 240 I = 1,K
00250      G(I,I) = G(IQ2,I) - G(IQ1,I)
00251      G(I,IC1) = G(I,IQ2) - G(I,IQ1)
00252      G(I,IC2) = G(I,IQ3)
00253      G(I,IQ1) = G(IQ2,IQ2) - G(IQ1,IQ2) - G(IQ2,IQ1)
00254      G(IQ1,IQ2) = G(IQ2,IQ3) - G(IQ1,IQ3)
00255      IF (HP) G(IQ1,IQ2) = G(IQ1,IQ2) + ENN
00256      GO TO 240
00257      230 DO 240 I = 1,K
00258      G(I,I) = 1.0
00259      240
00260      237 DO 240 I = 1,K
00261      G(I,I) = 1.0
00262      240

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MATX0055      000323
MATX0056      000326
MATX0057      000334
MATX0058      000344
MATX0059      000346
MATX0060      000362
MATX0061      000364
MATX0062      000372
MATX0063      000376
MATX0064      000403
MATX0065      000403
MATX0066      000407
MATX0067      000453
MATX0068      000454
MATX0069      000462
MATX0070      000465
MATX0071      000471
MATX0072      000477
MATX0073      000501
MATX0074      000505
MATX0075      000520
MATX0076      000527
MATX0077      000537
MATX0078      000537
MATX0079      000543
MATX0080      000545
MATX0081      000562
MATX0082      000606
MATX0083      000606
MATX0084      000606
MATX0085      000612
MATX0086      000623
MATX0087      000623
MATX0088      000625
MATX0089      000630
MATX0090      000630
MATX0091      000636
MATX0092      000641
MATX0093      000641
MATX0094      000656
MATX0095      000665
MATX0096      000672
MATX0097      000677
MATX0098      000677
MATX0099      000704
MATX0100      000707
MATX0101      000721
MATX0102      000757
MATX0103      000761
MATX0104      000764
MATX0105      000767
MATX0106      000774
MATX0107      001001
MATX0108      001007
MATX0109      001011

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001023
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001031
001106

MATX0090

240 G(1,IQ1) = G(1,IQ2)
260 KMAT = IMAT
IMAT = IMAT - 1
RETURN
END

001021
001023
001024
001025
001026
001027

END FOR

ORIGINAL PAGE IS
OF POOR QUALITY

FORM 5 LLWIS-00114-15-0011
 05A L: -10/25/79-17:39:20 (2,1)

SUBROUTINE OUT1 ENTRY POINT 001137
 0012 ENTRY POINT 001142
 0013 ENTRY POINT 001145

STORAGE USED: C00L11 001150; DATA01 000226; BLANK COMMON(2) 000000

COMMON BLOCKS:

C004 CONSTS 000006
 C009 POLCOM 000010
 C005 POINTS 000335
 C006 SPECES 012120
 C007 MISC 001264
 C010 TABA 000041
 C011 PERP 000166
 C012 GUP1 000073
 C013 CCC 000003

LATERAL REFERENCES (BLOCK, NAME)

C014 VAREPT
 C015 M00US
 C016 L1015
 C017 N1023
 C020 N1035
 C021 S0MT
 C022 NEPR34

STORAGE ASSIGNMENT (BLOCK, TYPE, RELATIVE LOCATION, NAME)

C000	C00103 IF	C001	000034 10L	0001	000025 1426	000043 1526	0001	000625 160L
C001	000112 1606	0001	000651 170L	0001	000657 175L	000726 177L	0001	000764 179L
C001	000766 180L	C000	000062 20F	0001	001041 200L	001076 210L	0001	001100 211L
C001	000175 2236	0001	000205 2306	0000	000037 240F	000233 2416	0001	000256 2536
C001	000264 2606	C001	000303 2706	0001	000313 2766	000112 280F	0000	000126 290F
C001	000003 30L	C000	000154 300F	0001	000332 3066	000156 310F	0001	000340 3136
C000	000122 320F	C001	000356 3226	0001	000402 3366	000116 340F	0001	000423 3476
C001	000444 3606	0001	000452 3656	0001	000467 3746	000506 4046	0001	000516 4126
C001	000542 4226	0001	000602 4416	0001	000605 4446	000065 45L	0001	000613 4516
C001	000636 4626	0001	000645 4676	0001	000201 50L	000664 5016	0001	000723 5126
C001	000754 5246	0001	001002 5466	0001	001014 5516	001036 5606	0001	001067 5726
C000	000111 60F	C006	000034 A	0011	000150 AFAT	000570 AM	0007	000624 AM
C007 F	000741 240M	C013	000133 AFP	0003 R	000000 AFMN	000004 ATOM	0007	000502 BU
C007	000521 60F	C010	000036 CALCH	0006	000000 COEF	000001 CONVL	0005 R	000032 CPR
C007	000625 64F1	0007	000564 CFSUM	0007	000604 DATA	005670 DELN	0013	000002 DEMAND
C007 R	001167 0145	0005 F	000064 ULVPT	0005 R	000047 ULVTP	002734 EN	0004	000000 EMO
C006	005364 64L6	0007	001263 ENLSAV	0007	000000 ENN	001261 ENNL	0007	001262 ENSAVE
C007 R	001073 6414	0011 L	000165 ECL	0007 R	000566 EORAT	000002 FA	0012 R	000003 FAF
C007 R	001114 64L	0012 L	000005 FL	0012	000006 FC	000007 FCP	0012	000012 FCSI

00001	000014	FCV	0012	000015	F6	0012	000017	FGE	0012	000020	FGV	0012	R	000021	FM		
00002	000023	FI	0012	000025	FTV	0012	R	000027	FM	0012	R	000031	FMT	0012	000032	FN	
00003	000052	FOUR	0017	I	001150	FOX	0012	000053	FP	0000	R	000036	FPC	0012	000054	FS	
00004	000056	F5V	0017	R	000057	FI	0012	R	000061	FTM	0012	R	000063	FV	0012	000065	FVEL
00005	000001	FVLM	0012	R	000003	F13	0012	000000	F9X	0005	R	000101	GAMMAS	0004	000001	GAS	
00006	000001	GNET	0013	R	000000	GRAPH	0000	R	000003	HEAD	0010	000003	HP	0007	000572	HPP	
00007	000567	H50R0	0015	R	000000	H50M	0006	005524	HO	0000	I	000035	I	0010	000030	IC	
00008	000000	IDR0U6	0014	000002	IE	0010	000015	IMAT	0010	000016	IOI	0010	000005	ISV	0010	000034	IT
00009	011444	I0SE	0010	000037	I0SAVE	0000	I	000034	J	0010	000026	JI10	000001	J0UT	0013	000001	JOUT
00010	000025	J50L	0010	000031	J51	0000	I	000032	K	0010	000014	KMAT	0004	I	000004	LANK	
00011	000463	LLMT	0010	000040	L5AVE	0000	I	000024	NC	0000	L	000006	MOLES	0000	I	000014	MM
00012	000026	NAME	0010	000017	NOF	0010	000033	NO	0010	000007	NP	0010	000011	NPT	0010	000035	NF2
00013	000012	NLM	0010	000013	N5	0000	I	000000	NSPPI	0010	000010	NT	0007	R	000565	OF	
00014	000027	NREAC	0010	I	000006	OX	0007	001227	OXF	0005	000016	P	0003	000002	PATH	000002	PATH
00015	000067	ONL	0004	I	001054	PECWT	0007	000563	PP	0005	R	000217	PFP	0003	R	000003	PBAR
00016	000000	PCP	0007	R	000574	RH	0007	R	001206	RHQP	0007	001207	RMW	0007	R	001131	PTEMP
00017	000005	RBR	0007	002570	S	0010	000033	SHOCK	0006	001754	SLN	0005	R	000251	SONVEL	0005	SONVEL
00018	000009	SV	0011	000047	SPIM	0005	R	000015	SSUM	0006	R	010770	SUB	0011	000101	SUBAR	
00019	000001	SUMN	0011	000116	SUPAR	0007	000003	S0	0005	000150	T	0006	011610	TEMP	0006	011610	TEMP
00020	002562	T0IGH	0012	000070	THREE	0007	001226	TLN	0007	000560	TLOW	0007	000557	TM	0007	000557	TM
00021	000561	T0ID	0005	R	000320	T0TN	0010	000002	T0	0007	000002	T1	0005	R	000266	T11	
00022	000071	TWO	0005	R	000202	V	0011	000064	VAC1	0005	R	000303	VLM	0007	000576	VMIN	
00023	000032	VMOG	0010	L	000032	VOL	0007	000600	VPLS	0005	R	000234	WM	0007	000602	WP	
00024	000025	YN	0006	R	000025	YX	0006	R	005524	Z	0004	000007	ZERO	0012	000072	ZERO	

[illegible]

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270 DIMENSION FVLM(2),HEAD(9),MW(2,2),YNI(5),YX(5),Z(10,3)
280 EQUIVALENCE (Z,MU)
290 INTEGER FOX,OX
300 LOGICAL EQL,MOLES,VOL
310
320 HEAD = (1XA6,2X51A2,F8.5,3X), 5X,F7.5,F13.3,4X,A1,F10.2,F9.4)
330
340
350
360 DATA HLAD/6H11XAG,,6H2X51A2,6H,F8.4,,6H3X), 5,6HX,F7.5,6H,F13.3,
370 1 6H,4X,A1,6H,F10.2,6H,F9.4)/,YN/6H2X11A2,6H2X21A2,6H2X31A2,
380 2 6H2X41A2,6H2X51A2/,YX/6H3X),5,6H3X),4,6H3X),31,6H3X),18,
390 3 6H3X), 5/,MW/24HMT FRACTION MOLES /,FVLM/12MVOLUME CC/G /
400
410
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COMMON /CCC/GRAPH,JOUT,DEMAND

IF (MOLES) K = 2

WRITE(JOUT,240) MW(1,M),MW(2,M)

FORMAT (77X,246,34H ENTHALPY STATE TEMP DENSITY/10X,

1 16HCHEMICAL FORMULA,65X,7HCAL/MOL,10X,6HDEG. M,3X,5HG/CM3)

DO 60 K = 1,NBLAC

IF (FOX(K) .NE. OX) GO TO 10

ND = 6-HOXIDNT

GO TO 50

10 ND = 6HFUEL

DO 40 J=1,5

40 IF (ANUM(K,J) .LE. U. .OR. NAME(K,J) .EQ. LANK) GO TO 45

J=6

45 J=J-1

HEAD(2) = YN(J)

HEAD(4) = YX(J)

60 WRITE(JOUT,HEAD) ND,(NAME(K,J),ANUM(K,J),I = 1,J),PECW(T(K),

ENTH(K),FAZ(K),RTEMP(K),DENS(K))

FPC = 100./(1.-OF)

WRITE(JOUT,20) OF ,FPC,EQRAT,RHOP

FORMAT (1H0,15X, 4HOF=, F8.4,4X,13HPERCENT FUEL=,F8.4,4X,

1 19HEQUIVALENCE RATIO= ,F7.4,4X,RHDENSITY=,F8.4/)

RETURN

ENTRY OUT2

VOLUME

FMT(3) = ONE

IF (NOT VOL) GO TO 50

CALL VAPMT(VLM,NPT)

WRITE(JOUT,FMT) FVLM,F8,(VLM(I), I = 1,NPT)

PRESSURE

50 GO 55 I = 1,NPT

55 V(I) = ATMNEPP(I)

CALL VAPMT(V,NPT)

WRITE(JOUT,FMT) FAP,F8,(V(I), I = 1,NPT)

TEMPERATURE

FMT(3) = F13

FMT(4) = 1-0

WRITE(JOUT,FMT) FTK,F8,(T(I), I = 1,NPT)

ENTHALPY

DO 75 J=1,NPT

75 V(J) = EBMHAP5U(I)

ORIGINAL PAGE IS
OF POOR QUALITY

```

002267 000267
002267 000267
000306 000306
000313 000313
000313 000313
000316 000316
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000340 000340
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000347 000347
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000625 000625
000655 000655
000655 000655
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000655 000655
000657 000657
000671 000671

      WRITE(JOUT,FMT) FM,FB,IV(I), J = 1,NPT)
      C ENTROPY
      FMT(4) = FOUR
      DO 76 I = 1,NPT
      76 V(I) = PHAR*SSUM(I)
      WRITE(JOUT,FMT) IS,FB,IV(I), J = 1,NPT)
      C DENSITY
      DO 70 I = 1,NPT
      70 IF (V(I) .GT. 0.0) V(I) = 1.0/V(I)
      WRITE(JOUT,1) (V(I), J = 1,NPT)
      1 FORMAT (1X,14DENSITY GZCC ,IP1SE9.3)
      WRITE(JOUT,80)
      80 FORMAT (1X,1)
      C MOLECULAR WEIGHT
      WRITE(JOUT,FMT) FM,FB,IV(I), J = 1,NPT)
      C (ULV/DLTP)
      IF (EQL) WRITE(JOUT,FMT) FT,FB,(DLVPT(I), J = 1,NPT)
      C (ULV/DLTP)
      IF (EQL) WRITE(JOUT,FMT) FV,FB,(DLVPT(I), J = 1,NPT)
      C HEAT CAPACITY
      DO 85 I = 1,NPT
      85 V(I) = PHAR*CPH(I)
      WRITE(JOUT,FMT) FCP,IV(I), J = 1,NPT)
      C GAMMA(S)
      WRITE(JOUT,FMT) FG,FB,(GAMMA(I), J = 1,NPT)
      C SONIC VELOCITY
      FMT(1) = TWO
      DO 95 I = 1,NPT
      95 SONVEL(I) = SONVELR*GAMMA(I)/T(I)/V(I)
      WRITE(JOUT,FMT) FSV,FVEL,(SONVEL(I), J = 1,NPT)
      RETURN
      C
      C ENTRY OUTS
      WRITE(JOUT,80)
      80 = 0
      C MOLE FRACTIONS EQUILIBRIUM OR FROZEN
      WRITE(JOUT,280)
      280 FORMAT (15HMOLE FRACTIONS/)
      IF (I.NOT. EQL) GO TO 175
      C EQUILIBRIUM MOLE FRACTIONS
      DO 170 I = 1,NPT
      170 V(I) = ENR(I)/TOTN(I)
      DO 150 I = 1,NPT
      150 IF (V(I) .GE. 5.0E-7) GO TO 160
      160 = 1
      DO 160 TO 170
      160 WRITE(JOUT,340) (SUBR(I), J = 1,3),FB,IV(I), I = 1,NPT)
      340 FORMAT (1X,3A4,2,IP1SE9.3)
      170 CONTINUE
      C OUTPUT COMPLETE GO EXIT
      GO TO 111
      C FROZEN MOLE FRACTIONS
      175 J = 0
      DO 179 I = 1,NPT
      179 V(I) = ENR(I)/TOTN(I)
      179 = 0

```


LINE	CODE	TEXT	ADDRESS
1390	000000	IF (V(0,1) .LT. 5.0E-7) ND = 1	000675
1400	000000	IF (V(0,1) .LT. 5.0E-7) GO TO 177	000700
1410	000000	OUTPUT VALUE ACCEPTED	000709
1420	000000	J = J + 1	000711
1430	000000	DO 176 I = 1,3	000719
1440	000000	176 Z(I,1) = SUM(R,1)	000723
1450	000000	177 IF (J .NE. 4 .AND. R .NE. NS) GO TO 179	000726
1460	000000	IF (J .EQ. 0) GO TO 180	000741
1470	000000	WRITE(JOUT,320) Z(1,1),Z(1,2),Z(1,3),V(1), I = 1,J	000743
1480	000000	FORMAT 11X,4(3H,F11.0,5X)	000762
1490	000000	J = 0	000762
1500	000000	179 CONTINUE	000766
1510	000000	180 IF (ND .EQ. 0) GO TO 211	000766
1520	000000	WRITE(JOUT,290)	000767
1530	000000	290 FORMAT 1/1X,116#ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHO	000774
1540	000000	156 MOLE FRACTIONS WERE LESS THAN 5.0E-7 FOR ALL ASSIGNED CONDITION	000774
1550	000000	25//)	000774
1560	000000	J = 0	000774
1570	000000	DO 210 K=1,NS	001002
1580	000000	DO 190 I=1,NPT	001010
1590	000000	190 IF (I*(R(I,1)/TOTN(1)) .GE. (5.0E-7)) GO TO 200	001020
1600	000000	J = J + 1	001027
1610	000000	DO 195 I = 1,3	001036
1620	000000	195 Z(I,1) = SUM(R,1)	001041
1630	000000	200 IF (J .NE. 10 .AND. R .NE. NS) GO TO 210	001050
1640	000000	IF (J .EQ. 0) GO TO 211	001056
1650	000000	WRITE(JOUT,300) Z(1,1),Z(1,2),Z(1,3), I = 1,J	001079
1660	000000	FORMAT 110(1X,24X)	001079
1670	000000	J = 0	001079
1680	000000	210 CONTINUE	001100
1690	000000	211 IF (I.NPT. MOLES) WRITE(JOUT,310)	001100
1700	000000	310 FORMAT 1/1X,77#NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND 0	001106
1710	000000	IF OXIDANT IN TOTAL OXIDANTS)	001106
1720	000000	RETURN	001106
1730	000000	END	001147
1740	000000	OUTPUT137	001147

FOR 5 UNITS-BLACT,LEWIS-REACT
 USA LS -10/25/79-17:19:27 III.1

SUBROUTINE REACT ENTRY POINT 000714

STORAGE USLU: C00L111 000730; DATA(0) 000167; BLANK COMMON(2) 000000

COMMON BLOCKS:

0003 HOLCON 000010
 0004 MISC 001264
 0005 INDA 000041
 0006 CCC 000003

LATENTIAL REFERENCE :BLOCK, NAME)

0007 PHEAD
 0010 NETA
 0011 NADDA
 0012 NETA
 0013 NETA
 0014 NETA
 0015 NETA

STORAGE ASSIGNMENT :BLOCK, TYPE, RELATIVE LOCATION, NAME)

0000	000107	107	0001	000256	101L	0001	000003	1216	0001	00013	1326	0001	000053	1546
0001	000104	176	0001	000040	20L	0001	000355	200L	0000	000110	21F	0001	000414	210L
0002	000551	218L	0001	000553	220L	0001	000615	222L	0001	000620	224L	0001	002635	226L
0003	000657	224L	0001	000652	230G	0001	000673	230L	0001	000172	236G	0001	000205	245G
0004	000227	260G	0001	000626	303G	0001	000123	31F	0001	000371	321G	0001	000411	335G
0005	000932	344G	0001	000475	355G	0001	000155	37L	0001	000525	370G	0001	000601	405G
0006	000504	410G	0001	000625	426G	0001	000650	441G	0001	000217	45L	0001	000663	450G
0007	000024	46L	0001	000240	50L	0004	000570	AM	0004	000624	AM	0004	000626	ANAME
0008	000741	480M	0004	000004	ATOM	0004	000502	80	0004	000521	80N	0005	000036	CALCH
0009	000001	480M	0004	000625	CPH	0004	000564	CPSUM	0004	000604	DATA	0006	000002	DEMAND
0010	001167	485N	0003	000000	END	0004	001263	ENLSAV	0004	000000	ENN	0004	001261	ENML
0011	001262	ENSAVE	0004	001073	ENTH	0004	000566	EQRAY	0004	001112	FAZ	0004	001150	FOX
0012	000001	945	0006	000000	GRAPH	0005	000003	HP	0004	000572	HPP	0004	000567	HSURU
0013	000102	I	0005	000030	IC	0005	000000	IOEBS	0003	000002	IE	0005	000015	IMAT
0014	000144	INJPA	0005	000075	IO	0005	000023	ION5	0005	000021	IP	0005	000037	IOSAVE
0015	000016	I21	0005	000005	ISV	0005	000034	IT	0003	000003	IZERU	0005	000077	J
0016	000102	JJ	0005	000026	JL1Q	0006	000001	JOUT	0005	000025	J50L	0005	000031	J51
0017	000076	K	0005	000014	KMAT	0005	000012	L	0003	000004	LANK	0004	000463	LLMT
0018	000020	LLH5	0005	000040	LSAVE	0003	000005	MOL	0000	000103	MOLE	0004	000006	MOLES
0019	000101	N	0004	000026	NAME	0005	000026	NC	0005	000022	NEW	0000	000100	NPHEL
0020	000005	NF2	0000	000000	NLS	0005	000017	NOF	0005	000020	NOMH	0005	000007	NP
0021	000011	NP1	0005	000027	NPLAC	0005	000013	NS	0005	000100	NT	0004	000565	OF
0022	000000	OF	0004	001227	OFF	0000	000106	PCMT	0004	000154	PECM	0004	000563	PP
0023	000574	PH	0004	001206	PHOF	0000	000104	PM	0004	0001207	PMW	0004	001131	RTIME
0024	000000	SHOF	0005	000033	SHOCK	0005	000004	SP	0004	000001	SUM4	0004	000003	SW
0025	000564	THIGH	0004	001276	TLN	0004	000540	TLUN	0004	000557	TM	0004	000561	TMIN

0005 000032 VOL

0004 R 000576 VMIN

0000 R 000001 V
0003 I 000007 ZER0

0004 000002 TT
0004 R 000002 WP

0004 000002 IF
0004 R 000000 VPLS

```
00101 10 SUBROUTINE REACT(FIRST)
00102 20 COMMON /HOLCON/ END,GAS,IE,I,ZERO,LANK,MOL,OX,ZERO
00103 30 COMMON /MISC/ ENN,SUPN,IT,SU,ATOM(3,10),LLMT(15),BO(15),
00104 40 HOP(15,2),TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,
00105 50 MSUBO,AM(2),HPP(2),RH(2),VMIN(2),VPLS(2),WP(2),
00106 60 DATA(16),AM1,CPRI,NAME(15,5),ANUM(15,5),PECUT(15),
00107 70 ENTH(15),FAZ(15),RTIMP(15),FOX(15),DENS(15),RHOP,
00108 80 MM(15),ILN,OXF(26),ENNL,ENSAVE,ENLSAV
00109 90 COMMON /INDX/ IOLBUG,CONVG,TP,HP,SP,ISV,MOLES,MP,NT,NPT,L,NS,
00110 100 KMAT,IMAT,IOI,NOF,NOMIT,JP,NEWB,IONS,NC,JSOL,JLIQ,
00111 110 NREAC,JC,JSI,VOL,SHOCK,IT,NFZ,CALCH,ISAVE,LSAVE
00112 120
00113 130 COMMON /CLC/ GRAPH,JOUT,DEMAND
00114 140
00115 150 DATA NLSZ/0/
00116 160 DIMENSION ANAME(15,5),V(15),LLMTS(15),SBOPI(15,2)
00117 170 EQUIVALENCE (NAME,ANAME)
00118 180 INTEGER FOX,OX,ZERO
00119 190 LOGICAL MOLES,NEWB
00120 200
00121 210 LOGICAL FIRST
00122 220 DATA IOI/8/
00123 230
00124 240 DO R R = 1,2
00125 250 WPMK=0.
00126 260 HPP(K)=0.
00127 270 RH(K)=0.
00128 280 VPLS(K)=0.
00129 290 VMIN(K)=0.
00130 300 AMIN(K)=0.
00131 310 DO R J=1,15
00132 320 LLMT(J)=0
00133 330 HOP(J,K) = 0.0
00134 340 NFUEL = 0
00135 350 N=1
00136 360 L=1
00137 370
00138 380 CALL SUBROUTINE TO SET UP REACTANTS ON FILE R
00139 390 CALL REAU(FIRST)
00140 400
00141 410 READ REACTANTS FROM FILE R
00142 420 REWIND IO
00143 430 READ(10,10) NREAC
00144 440
00145 450 FORMAT(13)
00146 460
00147 470 CONTINUE
00148 480 READ(9,21) (NAME(I,1),ANUM(I,1),I=1,5),PECUT(I),MOLE,ENTH(I),FAZ(I)
00149 490 I = I+1,FOX(I),DENS(I)
00150 500 FORMAT(2X,5A2,F8.4,2X1,/,F10.6,2X,A1,F13.4,4X,A1,F12.3,
00151 510
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```
510 00170 1 3X,A1,I12.5,1X1
520 00171 IF (NAMEIN,1).EQ.0) GO TO 200
530 00172 IF (L.EQ.0) GO TO 20
540 00173 WRITE(JOUT,31)NAMEIN,1,ANUMIN,1,I=1,5,PECMIN,MOLE,ENTHIN,
550 00174 *ITERJOUT,31)NAMEIN,1,ANUMIN,1,I=1,5,PECMIN,MOLE,ENTHIN,
560 00175 1 FZIN,STEPIN,FOXIN,DENSIN
570 00176 31 FORMAT(1X,5I2,F8.4,2X),F10.6,2X,A1,F11.4,2X,A1,F10.3,2X,A1,F11.5)
580 00177 IF (MOLE.EQ.0) MOLE = .TRUE.
590 00178 IF (OXIDANT, K = 1: IF FUEL, K = 2:
600 00179 IF (FOXIN).EQ.0) FOXIN = 0X
610 00180 IF (PECMIN).LE. 0.0) PECMIN = 1.0
620 00181 K = 1
630 00182 IF (FOXIN).EQ.0) GO TO 37
640 00183 K = 2
650 00184 MFUEL = MFUEL+1
660 00185 37 DO 38 J=1,15
670 00186 38 DATA(J) = 0.0
680 00187 AMED.
690 00188 DO 100 JJ=1,5
700 00189 IF (ANUMIN, JJ) .EQ. 0.0) GO TO 101
710 00190 IF (NAMEIN, JJ) .EQ. 0.0) NAMEIN, JJ) = 0X
720 00191 DO 43 J=1,15
730 00192 I = J
740 00193 IF (LIMIT(J).EQ.0) GO TO 45
750 00194 41 IF (NAMEIN, JJ) .EQ. LIMIT(J)) GO TO 46
760 00195 45 L = 1
770 00196 LLIMIT(J)=NAMEIN, JJ)
780 00197 46 DO 48 J = 1,101
790 00198 48 IF (ATOM(I,1) .EQ. ANAMEIN, JJ)) GO TO 50
800 00199 L=0
810 00200 GO TO 40
820 00201 50 KM = RM + ANUMIN, JJ)*ATOM(I,1)
830 00202 VIJ) = ATOM(I,1)
840 00203 100 DATA(J) = ANUMIN, JJ)
850 00204 101 PCMT=PECMIN
860 00205 PCMT=PCMT+PCMT*RM
870 00206 MPIN)=MPIN) + PCMT
880 00207 IF (NAMEIN,5) .NE. IZER0) HPPIN) = HPPIN) + ENTHIN*PCMT/RM
890 00208 AMIN)=AMIN)+PCMT/RM
900 00209 DO 110 J=1,L
910 00210 110 BOP(J,K) = DATA(J)*PCMT/RM + BOP(J,K)
920 00211 IF (DENSEIN).GT. 0.0) BHIK) = BHIK) + PCMT/DENSEIN)
930 00212 KM=KM + RM
940 00213 N = N+1
950 00214 IF (N.NE.14) GO TO 20
960 00215 200 NREAL=N-1
970 00216 IF (FUEL.EQ.0) GO TO 210
980 00217 103 PERCENT OXIDANT, CALL REACTANTS FULL
990 00218 DO 205 N=1,NREAL
1000 00219 FOXIN) = FOXIN)
1010 00220 BHIK) = BHIK)
1020 00221 AMIN) = AMIN)
1030 00222 HPPIN) = HPPIN)
1040 00223 BHIK) = BHIK)
1050 00224 205 N=1, NREAL
1060 00225 206 N=1, NREAL
```

```

1034      DO 204 J=1,L
1035      BOP(J,2) = BOP(J,1)
1036      IF (L.EQ. 0) RETURN
1037
1038      DO 240 K=1,2
1039      IF (BPK(K).LE. 0.0) GO TO 220
1040
1041      HPP(K)=HPP(K)/WP(K)
1042      AM(K) = WP(K)/AM(K)
1043
1044      IF (RH(K) .GT. 0.0) RH(K) = WP(K)/RH(K)
1045
1046      DO 215 J=1,L
1047      BOP(J,1)=BOP(J,K)/WP(K)
1048      IF (V(J).LT.0.0) VMIN(K) = VMIN(K)+BOP(J,K)*V(J)
1049      IF (V(J) .GT. 0.0) VLS(K) = VLS(K) + BOP(J,K)*V(J)
1050      IF (MULS) GO TO 220
1051
1052      DO 218 N=1,NREAC
1053      IF ((FOXIN).EQ.0X.AND.K.EQ.2).OR.(FOXIN).NE.0X.AND.K.EQ.1)UOT0218
1054      PECNT(N) = PECNT(N)/WP(K)
1055
1056      218 CONTINUE
1057      220 CONTINUE
1058
1059      NEWR=.TRUE.
1060      C AME ELEMENTS SAME AS FOR LAST SET OF REACTANTS, IF SO, NEWR=.FALSE. 4/23/70
1061      IF (L.NE. NLS .OR. NOMIT .NE. 0) GO TO 226
1062
1063      DO 224 I=1,NLS
1064      DO 222 J=1,L
1065      IF (LLMT(I).NE.LLMTS(I)) GO TO 222
1066      SBUP(I,1) = BOP(J,1)
1067      SBUP(I,2) = BOP(J,2)
1068      GO TO 224
1069
1070      222 CONTINUE
1071      GO TO 226
1072
1073      224 CONTINUE
1074      NEWR = .FALSE.
1075      DO 225 I = 1,L
1076      LLMT(I) = LLMTS(I)
1077      BOP(I,1) = SBUP(I,1)
1078      BOP(I,2) = SBUP(I,2)
1079      GO TO 229
1080
1081      225 BOP(I,2) = SBOP(I,2)
1082
1083      246 NLS = L
1084      NOMIT = 0
1085      NEWIND = 0
1086      DO 228 I = 1,L
1087      SBUP(I,1) = BOP(I,1)
1088      SBUP(I,2) = BOP(I,2)
1089      LLMTS(I) = LLMT(I)
1090      228 LLMTS(I) = LLMT(I)
1091      229 DO 230 N=1,NPLAC
1092      IF (GENS(N) .GT. 0.0) GO TO 230
1093      RH(I) = 0.
1094      HP(I) = 0.
1095      RETURN
1096
1097      233 CONTINUE
1098      RETURN
1099      END

```

PCIN0111

4/23/70

JOHN S LEWIS, RMTOUT, LEWIS, RMTOUT
 11 A 13 -10/25/79-17:39:33 (9.1)

SUBROUTINE RMTOUT ENTRY POINT 000521

STORAGE USED: C00111 000530; DATA(0) 000120; BLANK COMMON(2) 000000

COMMON BLOCKS:

C0013 CONSTS 000006
 C0014 POINTS 000335
 C0015 SPELES 012120
 C0016 INDX 000041
 C0017 PERF 000166
 C0018 OPT 000073
 C0019 CCC 000003

EXTERNAL REFERENCES (BLOCK, NAME)

0012 OUT1
 0013 VARPMT
 0014 OUT2
 0015 GAMLEFF
 0016 OUT3
 0017 N=0013
 0018 M1013
 0019 M1013
 0020 SORT
 0021 M1013
 0022 M1013
 0023 M1013
 0024 M1013

STORAGE ASSIGNMENT (BLOCK, TYPE, RELATIVE LOCATION, NAME)

0001 000057 1446 0000 000066 150F 0001 000070 152G
 0002 000176 200L 0000 000075 208F 0001 000231 220G
 0003 000312 252G 0001 000334 264G 0001 000344 272G
 0004 000412 317G 0001 000423 324G 0001 000441 335G
 0005 000006 37F 0000 000027 38F 0000 000056 40F
 0006 000150 ALAT 0007 000133 APP 0003 000000 ATMN
 0007 000000 COEF 0006 000001 CONVG 0000 000032 CPH
 0008 000002 DEFHAND 0004 000064 ULVPT 0004 000047 ULVTP
 0009 000165 LUL 0000 000002 FA 0010 000003 FAP
 0010 000007 ICE 0010 000012 FCST 0010 000014 FCV
 0011 000000 FGV 0010 000021 FH 0010 000023 FI
 0012 000031 FMT 0010 000050 FN 0010 000052 FOUR
 0013 000056 FSV 0010 000057 FT 0010 000061 FTK
 0014 000001 F13 0010 000000 F9X 0004 000101 GAMMAS
 0015 000003 HP 0004 000000 HSUM 0005 000524 HN
 0016 000000 ICHROL 0006 000015 IMAT 0000 000103 INJPS
 0017 000037 ICSAVE 0006 000016 ICI 0006 000005 ISV
 0018 000026 JULQ 0011 000001 JOUT 0006 000025 JSOL
 0019 000014 MAT 0006 000040 LSAVE 0006 000006 MOLES

0001 000115 166G 0001 000144 176G
 0002 000416 220L 0001 000257 234G
 0003 000362 303G 0001 000505 312L
 0004 000462 346G 0001 000501 356G
 0005 000047 737F 0005 006034 A
 0006 000002 AM 0006 000036 CALCH
 0007 000005 CSIR 0006 000670 DELM
 0008 002734 LN 0005 005360 EMLN
 0009 000005 FB 0010 000006 FC
 0010 000015 FG 0010 000017 FGE
 0011 000025 FIV 0010 000027 FM
 0012 000053 FF 0010 000054 FS
 0013 000063 FV 0010 000065 FVEL
 0014 000001 GMLT 0010 000000 GRAPH
 0015 000004 I 0006 000030 IC
 0016 000023 IONS 0006 000021 IP
 0017 000034 IT 0006 011444 IUSE
 0018 000031 JSI 0000 000003 K
 0019 000024 NC 0006 000022 NEWP


```

00156      C      PRESSURE RATIOS
00157      FMT(3) = ONE
00158      CALL VARFMT (APP,NPT)
00159      WRITE(JOUT,FMT) FP,FB,FB,(APP(1)), I = 1,NPT)
00160      CALL OUT2
00161      IF (NPT .LT. 2) GO TO 312
00162      DO 202 K=2,NPT
00163      SPIM(K) = SORT(2,UORBB*(HSUM(1)) - HSUM(K))/GMET
00164      AM = (A/W) IN UNITS OF SEC/ATH
00165      AM = RRR*TTIM/(PPP(K)*HMM(K)*SPIM(K)*GMET**2)
00166      IF (K.NL*2)GO TO 200
00167      CSTR = GMET*AM*PPP(1)
00168      ACAT(2) = 1.
00169      200 VACI(K)=SFIM(K)*PPP(K)*AM
00170      IF (SONVEL(K) .GT. 0.0) VMOC(K) = GMET*SPIM(K)/SONVEL(K)
00171      V(1) = 0.0
00172      WRITE(JOUT,FMT) FGV,FVEL,(V(1)), I = 1,NPT)
00173      C      MACH NUMBER
00174      FMT(4) = FOUR
00175      VMOC(1)=0.
00176      IF (GAMMA(2) .LE. 0.0) VMOC(2) = 0.0
00177      WRITE(JOUT,FMT) FN,FB,(VMOC(1)), I = 1,NPT)
00178      WRITE(JOUT,208)
00179      208 FORMAT (1H )
00180      C      AREA RATIO
00181      CALL VARFMT (ALAT,NPT)
00182      FMT(3) = F9X
00183      WRITE(JOUT,FMT) FA,FB,FB,(ALAT(1)), I = 2,NPT)
00184      C      CSTAR
00185      FMT(4) = F13
00186      FMT(5) = TWO
00187      WRITE(JOUT,FMT) FCST,FB,(CSTR, I = 2,NPT)
00188      C      CF - THRUST COEFFICIENT
00189      FMT(5) = FOUR
00190      DO 212 I=2,NPT
00191      V(1) = GMET*SPIM(1)/CSTR
00192      WRITE(JOUT,FMT) FC,FB,FB,(V(1)), I = 2,NPT)
00193      IF (IGAM .EQ. 0) GO TO 220
00194      C      EFFECTIVE GAMMA
00195      CALL GAMEFF (V,GAMMA,APP,NPT,HO)
00196      WRITE(JOUT,FMT) FGI1,FGE,FB,(HO(1)), I = 2,NPT)
00197      C      VACUUM THRUST COEFFICIENT
00198      220 DO 230 I = 2,NPT
00199      V(1) = GMET*VACI(1)/CSTR
00200      WRITE(JOUT,FMT) FCV,FB,FB,(V(1)), I = 2,NPT)
00201      C      VACUUM IMPULSE
00202      FMT(5) = THREE
00203      WRITE(JOUT,FMT) FIV,FB,(VACI(1)), I = 2,NPT)
00204      C      SPECIFIC IMPULSE
00205      WRITE(JOUT,FMT) FI,FB,(SPIM(1)), I = 2,NPT)
00206      C      FROZEN MOLE FRACTION OUTPUT MOVED TO SUBROUTINE OUT3
00207      312 CALL OUT3
00208      RETURN
00209      END

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WFOH15 LEWIS-ROCKET, LEWIS-ROCKET
NSA 15-10/25/79-17:39:40 (8.1)

SUBROUTINE HOCKET ENTRY POINT U01303

STORAGE USED: CODE(1) U01312; DATA(1) U00222; BLANK COMMON(2) U00000

COMMON BLOCKS:

U003 CONSTS U00006
U004 POINTS U00335
U005 MISC U01264
U006 INDX U00041
U007 PERF U00166
U010 CCC U00003

EXTERNAL REFERENCES (BLOCK, NAME)

U011 NEWOF
U012 FROZEN
U013 EQLBRM
U014 KATOUT
U015 SAVE
U016 MNLX
U017 MNLX
U020 XPRR
U021 N=003
U022 N1025
U023 AL06
U024 EXP
U025 XFUR
U026 SORT
U027 NLRR34

STORAGE ASSIGNMENT (BLOCK, TYPE, RELATIVE LOCATION, NAME)

U001	U00013	1256	U001	U00155	1332L	U001	U00030	1416	U001	000047	1536	U000	00076	1811F
U001	U00275	191L	U001	U00413	192L	U000	U00073	194F	U001	000254	195L	U001	000121	2006
U001	U00021	303L	U001	U00040	306L	U001	U00076	321L	U001	000115	322L	U001	000146	331L
U001	U00153	332L	U001	U00170	333L	U001	U00206	334L	U001	000603	799L	U001	000531	800L
U001	U00756	802L	U001	U00033	805L	U001	U00676	809L	U001	000646	810L	U001	001002	820L
U000	U00117	821F	U001	U001010	830L	U001	U01036	834L	U001	001046	835L	U001	001050	859L
U001	U01054	860L	U000	U00131	862F	U000	U00160	865F	U001	001114	870L	U001	001130	880L
U001	U00452	899L	U001	U00472	900L	U000	000065	923F	U001	000411	925L	U001	001164	920L
U001	U01225	997L	U001	U01257	999L	U007	U00150	ACAT	U000	000037	ACATL	U005	000570	AM
U005	U00624	AM1	U005	U00741	AMUM	U007	U00133	APP	U000	000035	APPL	U000	000033	APATIO
U000	U00003	APL	U000	U00001	ASQ	U003	U00000	ATHN	U005	000004	ATOM	U000	000030	AWI
U005	U00502	BU	U005	U00521	POP	U006	U00036	CALCH	U006	000001	CONVG	U004	000032	CPH
U005	U000023	CPWF	U005	U00625	CPH1	U005	U00564	CPSUM	U005	000604	DATA	U010	000002	DEMAND
U005	U01167	DFMS	U000	U00026	OH	U000	U00032	OLNP	U000	000040	OLNPL	U000	000027	OLT
U004	U00064	ULVFT	U004	U00047	ULVTF	U000	U00034	ELN	U005	001263	ENLSAV	U005	000000	ENH
U005	U0141	ENL	U005	U01264	ENLSAVE	U005	U01073	ENTH	U007	000165	FOL	U005	000566	FOPAT

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OF POOR QUALITY

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0005 001112 IAZ 0005 001150 FOX 0000 L 000006 FROZ 0004 R 000101 GAMMAS 000001 GME T
0010 000000 GRAPH 0006 L 000003 MP 0005 000572 HPP 0005 000567 HSUBU 000000 HSUM
0000 000012 I 0006 000030 IC 0000 I 000000 ICASE 0006 I 000000 IOERUG 0001 000011 IGAM
0006 000015 IMAT 0000 000206 INJPS 0000 I 000016 IOF 0006 000023 IONS 0006 I 000021 IP
0000 000022 IPF 0006 000037 IQSAVE 0006 000016 IQI 0000 I 000020 ISUB 0000 I 000021 ISUP
0006 000005 ISV 0006 I 000034 IT 0000 I 000017 ITNUM 0000 I 000025 ITROT 0006 000026 JLIQ
0010 000001 JOUT 0006 I 000025 JSOL 0006 000031 JSI 0006 000014 KMAT 0005 000463 LLMT
0006 000040 LSAVE 0006 000006 MOLES 0005 000626 NAME 0006 000024 NC 0006 000022 NEWR
0006 000035 NFZ 0006 000012 NLM 0006 I 000017 NOF 0006 000020 NOMII 0006 I 000007 NP
0000 000013 NPT 0006 I 000011 NPT 0006 000027 NREAC 0006 000013 NS 0000 I 000014 NSUB
0000 000015 NSUP 0006 I 000010 NT 0005 R 000565 OF 0005 R 001227 OXF 0004 R 000116 P
0003 000002 PATH 0007 R 000000 PCP 0000 R 000031 PCPLT 0005 001054 PECMI 0005 R 000563 PP
0004 R 000217 PPP 0003 000003 RBAR 0003 R 000004 RBR 0005 000574 RH 0005 001206 RHOP
0000 000041 RKTING 0005 001207 RMW 0006 001131 RIEMP 0003 000005 RVR 0000 L 000007 SEQL
0006 000033 SHOCK 0004 000251 SONVEL 0006 L 000004 SP 0007 000047 SPIH 0004 R 000150 T
0007 R 000101 SUBAR 0005 000001 SUMN 0007 R 000116 SUPAR 0005 R 000003 SO 0005 000557 TH
0000 L 000010 THI 0005 000562 THIGH 0005 001226 TLN 0005 000560 TLOW 0005 000557 TH
0000 R 000024 TMLT 0005 000561 TMID 0000 R 000036 TOL 0004 000320 TOTN 0006 L 000002 TP
0005 R 000002 TT 0004 R 000266 TTT 0000 D 000003 USQ 0004 000202 V 0007 000064 VACT
0004 R 000303 VLM 0005 000576 VMIN 0007 000032 VMOC 0006 000032 VOL 0005 000600 VPLS
0004 R 000234 WH 0005 000602 WP

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00101 10 SUBROUTINE ROCKET
00101 20 C
00101 30 C
00101 40 C
00103 50 COMMON /CONSTS/ ATMN,GMEI,PATH,RBAR,RBR,RVR
00104 60 COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),ULVTP(13),ULVPT(13)
00104 70 1 ,GAMMAS(13),PI(26),I(26),V(13),PP(13),WM(13),SONVEL(13),TT(13)
00104 80 2 ,VLM(13),TOTN(13)
00105 90 COMMON /MISC/ LNN,SUMN,TT,SO,ATOM(3,101),LLMT(15),BO(15),
00105 100 BOF(15,2),TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,
00105 110 HSUBO,AM(2),MPP(2),RM(2),VMIN(2),VPLS(2),WP(2),
00105 120 UDATA(6),AMI,CPR1,NAME(15,5),ANUM(15,5),PECM(15),
00105 130 ENTH(15),FAZ(15),RIEMP(15),FOX(15),DENSI(5),RHOP,
00105 140 RMW(15),TLN,OXF(26),LNNL,ENSAVE,ENLSAV
00106 150 COMMON /INDX/ IDEBUG,CONVG,TP,HP,SP,JSV,MOLES,MP,NT,NPT,NLM,NS,
00106 160 KMAT,THAT,IOI,NOF,NOMIT,IP,NEWR,IONS,NC,JSOL,JLIQ,
00106 170 NREAC,IC,JSI,VOL,SHOCK,IT,NFZ,CALCH,IOSAVE,LSAVE
00107 180 COMMON /PERF/ PCPI(26),VMOC(13),SPIM(13),VACT(13),SUBAR(13),
00107 190 SUPAR(13),APP(13),AEAT(13),EUL
00107 200 C
00110 210 COMMON /CCCC/ GRAPH,JOUT,DEMAND
00110 220 C
00111 230 DATA ICASE/0/
00113 240 DOUBLE PRECISION ASO,USO
00114 250 LOGICAL AREA,ECL,FROZ,HP,SEUL,SP,THI,TP
00114 260 C
00115 270 NAMELIST /RATING/ EUL,FROZ,IGAM,PCP,SUBAR,SUPAR
00115 280 C
00115 290 IF 2 = 1
00115 300 APT(1) = 1.
00117 310 IF ICASE .GT. 0) GO TO 303
00119 310

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101.2 320 ICASE = 1
101.3 330 IGAM = 0
101.4 340 UO 300 I=1,26
101.7 350 PCP112 = 0.
101.10 360 SUBAR11 = 0.0
101.12 370 EQL = .TRUE.
101.15 380 FROZ = .FALSE.
101.19 390 READ (J,PRTINP)
101.17 400 NPP = 0
101.21 410 UO 305 I = 1,26
101.24 420 IF (PCP11) .LE. 0.0) GO TO 306
101.27 430 NPP = 1
101.30 440 NPP = NPP*2
101.33 450 NSUB = 0
101.36 460 NSUP = 0
101.39 470 UO 320 I=1,13
101.42 480 IF (SUBAR11) .GT. 0.0) NSUB = NSUB + 1
101.45 490 IF (SUBAR11) .GT. 0.0) NSUP = NSUP + 1
101.48 500 WRITE(JOUT,PRTINP)
101.51 510 SEUL = EQL
101.54 520 IOF = 0
101.57 530 IT = 3400.
101.60 540 LOOP FOR EACH U/F
101.63 550 IT = 1
101.66 560 IOF = IOF + 1
101.69 570 UF = OAF(10F)
101.72 580 CALL NLMOF
101.75 590 IF (111) .LE. 0.0) GO TO 322
101.78 600 IT = 1111)
101.81 610 LOOP FOR CHAMBER PRESSURES
101.84 620 UO 998 IP = 1,NP
101.87 630 ITNUM = 0
101.90 640 ARLA = .FALSE.
101.93 650 IF (111) .LE. 0.0) HP = .TRUE.
101.96 660 IF (111) .GT. 0.0) TP = .TRUE.
101.99 670 SP = .FALSE.
102.02 680 EQL = .TRUE.
102.05 690 ISUB = 1
102.08 700 ISUP = 1
102.11 710 PP = P11P)
102.14 720 IFP = 1
102.17 730 LOOP FOR PRESSURE RATIOS
102.20 740 331 IF(ALL) GO TO 332
102.23 750 CALL FROZEN
102.26 760 GO TO 1332
102.29 770 332 CALL TOLBFM
102.32 780 IT = 0 IF NO CONVERGENCE
102.35 790 1332 IF (11) .GT. 0.0) GO TO 333
102.38 800 IF (NPT -LT. 2) RETURN
102.41 810 GO TO 900
102.44 820 333 IF (11P,GT.1) GO TO 195
102.47 830 COMUSTION, CHAMBER
102.50 840 LCL = JFQL
102.53 850 TP = .FALSE.
102.56 860 HP = .FALSE.
102.59 870 SP = .TRUE.
102.62 880
102.65 890
102.68 900
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RUCM0060
RUCM0062
RUCM0063
RUCM0064

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      SU = SUM(I1)
      CPPI = CFSUM
      234 TMELT = 1.
      ITROT = 3
      ITH = .FALSE.
      APP(2) = (GAMMA5(1)+1.1/2.1)*(GAMMA5(1)/(GAMMA5(1)-1.1))
      IF (I1) WRITE(JOUT,194) APP(2)
      PP = PP(1)/APP(2)
      IT = 2.011/(GAMMA5(1)+1.1)
      ISV = 1
      GO TO 870
195 USQ = 2.04888*(HSUM(1) - HSUM(IMP1))
      IF (I1) GO TO 900
      ITHROT =
      IF (I1) ITH = GO TO 191
      GAMMA5(2) = U.
      GO TO 899
191 ASQ = HBR*(GAMMA5(2)+1.0)*ENN
      IF (I1) USQ = EQ.1.0R.10EBUG.EQ.2) WRITE(JOUT,923)USQ,ASQ
      923 FORMAT(SHUSQ=,15.8,5X,4MASQ=,E15.8)
      USQ = (USQ-ASQ)/ASQ
      IF (I1) LT.0.1) DH=-DH
      IF (I1) LE.0.4E-4.0H.1TROT.EQ.U) GO TO 699
      IF (I1) SOL. ME. U) GO TO 925
      IF (I1) TMELT. LE. U.0) GO TO 192
      ULT = ALG(1)TMELT/IT)
      PP = PP*EXP(ULT*CPPI(2)/(ENN*ULT*VP(2)))
      APP(2) = PP(1)/PP
      ITH = .TRUE.
      GO TO 331
      925 TMELT = IT
192 APP(2) = APP(2)/(1.0 + (USQ - ASQ)/(ENN*(GAMMA5(2) + 1.0)*HBR*IT))
      PP = PP(1)/APP(2)
      ITROT = ITROT-1
      IF (I1) WRITE(JOUT,194) APP(2)
194 FORMAT(7H PC/PT=,F9.6)
      GO TO 331
      899 AMT = ENN*IT/(PP*USQ**0.5)
      PCPLT = ALG(1)APP(2)
      920 ISV = 0
      IF (I1) LF. U.0) GO TO 860
      ALAT(IMP1) = ENN*IT/(PP*USQ**0.5*AMT)
      IF (I1) AREA) GO TO 800
      IF (I1) PP.LT.MPF) GO TO 859
      IF (I1) SUB.IMP1.EQ.U) GO TO 860
      AREA = .TRUE.
      PCP ESTIMATES FOR AREA RATIOS
      800 IF (I1) NUM.ME.U) GO TO 810
      OLMT = 1.
      ITNUM = 1
      AREA10 = SUBAR(1SUB)
      IF (I1) SUB. LE. U) AREA10 = SUBAR(1SUB)
      ELA = ALG(1)AREA10
      IF (I1) SUB. LE. U) GO TO 799
      APP(2) = FCPLT/(SUBAR(1SUB)+1.0.5*7*ELN**0.9.95*OLMT)
      IF (I1) AREA10.LT.1.0) APP(2) = 9.9*APP(2)

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ROCK0066

ROCK0073

ROCK0079

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ROCKU088

ROCKU121

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1449      GO TO 859
1450      799 IF (ISUP*ITSUP).LT.2.) GO TO 805
1451      IF (ISUP.GT.1.AND.SUP*ITSUP-1).GE.2.) GO TO 802
1452      APPL = GAMMA*23*ELN*1.4
1453      GO TO 859
1454
1455      805 APPL = SUP*ITSUP*(1.535-3.294*ELN))*PCPLT
1456      GO TO 859
1457
1458      810 IF (IDBUG.LE.0) NPT.LT. IDBUG) GO TO 809
1459      *RITELCOUT,1811*ITNUM,ARATIO,ARATIO,APP(NPT),DLNP
1460      1811 FORMAT (6HITELC=12,5X,15HASSIGN=0 ARAT=,F15.8,5X,6HAR/AT=,F15.8,
1461      15X,5HPCPLT=,F15.8,5X,11HDELTA (N P=,F15.8)
1462      809 TOL = 1.0E-5
1463      IF (ARATIO.GE. 10.0) TOL = 4.0E-5
1464      IF (AR*ARATIO.NPT) - ARATIO)/ARATIO .LT. TOL) GO TO 810
1465      IF (AR*DLNP.LT. 4.0E-6) GO TO 810
1466      ARATL = ALG*ARATIO(NPT)
1467      I*NUM = ITNUM + 1
1468      IF (ITNUM.GT. 25) GO TO 820
1469      ASQ = HRR*GAMMA*INPT)*ENN*TT
1470      DLNPL = GAMMA*INPT)*USQ/(USQ-ASQ)
1471      802 DLNP = DLNPE*ELN-DLNPE*ARATL
1472      APPL = APPL + DLNP
1473      IF (ITNUM.EQ.1) GO TO 859
1474      APP(NPT) = EXP(APPL)
1475      PP = PCPLT/APP(NPT)
1476      GO TO 531
1477
1478      820 *RITELCOUT,821) ARATIO
1479      821 FORMAT (7IUX,NOHROCKET DID NOT CONVERGE FOR AREA RATIO =,F11.6/)
1480      830 ITNUM = 0
1481      ARATIO(NPT) = ARATIO
1482      IF (NSUB.LE.0) GO TO 834
1483      ISUP = ISUP+1
1484      IF (ISUB.LE. NSUB) GO TO 800
1485      ISUB = 1
1486      NSUB = -NSUB
1487      IF (ISUP.LE.NSUP) GO TO 800
1488      GO TO 835
1489      834 ISUP = ISUP+1
1490      IF (ISUP.LE.NSUP) GO TO 800
1491      ISUP = 1
1492      AREA = .FALSE.
1493      835 GO TO 860
1494      859 ISV = NPT
1495      IF (NPT.NE.13) GO TO 870
1496      CALL RKTOUT (IGAM)
1497      IF (IT.LE. 0.0) ISV = 0
1498      IF (C*U1.EQL.AND. 11 .LE. U.0) *RITELCOUT,862)
1499      862 FORMAT (7/2X,17SHCALCULATIONS WERE STOPPED IN ROCKET BECAUSE NEXT
1500      POINT IS MORE THAN 50 DEGREES BELOW TEMPERATURE RANGE OF A CONDENS
1501      *ED SPECIES)
1502      IF (ISV.EQ.0) GO TO 990
1503      IDBUG = IUEH0-13
1504      *RITELCOUT,865)
1505      865 FORMAT(1H1)
1506      *PT = C
1507      870 *PT = NPT + 1
1508
1509      14554
1510      003.5
1511      003.7
1512      003.1
1513      003.2
1514      003.3
1515      003.4
1516      003.5
1517      003.6
1518      003.7
1519      003.76
1520      003.77
1521      003.86
1522      004.02
1523      004.04
1524      004.07
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ROCKU129

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IF (.NOT. EQL) GO TO 880
IF (ISV.EQ.1) ISV = -1
CALL SAVE
880 IPP = IPP+1
IF (IPP.EQ.2) GO TO 331
IF (.NOT. EQL) APP(IPP)=PCP(IPP-2)
IF (APP(IPP)=EXP(1))
PF = PCP(IPP)/APP(IPP)
GO TO 331
990 IF (IOFBUG.LT.0) IOFBUG=IOFBUG+13
IF (NSUB.LT.0) NSUB=-NSUB
IF (.NOT. FROZ.OR..NOT. EQL) GO TO 997
CPH(1) = CPH
GAMMA(1) = (CPH/ICPH-1./MM(1))
IT = IT+1
IPP = 1
MPI = 1
CALL SAVE
EQL = .FALSE.
END = 1./MM(1)
GO TO 334
997 MPI = 1
WRITE(JOUT,865)
IF (EQL) CALL SAVE
IT = IT+1
IF (IT.GE.N1) GO TO 999
IT = IT+1
IT = IT+1
GO TO 322
999 IF (IOF.GE. NOF) RETURN
END

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10974 2019
10975 2029
10976 2039
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11005 2329

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00005 LEWIS-RELAB,LLWIS-RELAB
 00006 13-10/5/79-17:32:49 117.1

SUBROUTINE READ ENTRY POINT 001255

STORAGE USED: CODE(1) 001273; DATA(0) 001031; BLANK COMMON(2) 000000

EXTERNAL REFERENCES (BLOCK, NAME)

00005 MVELS
 00006 PAGE11
 00007 CHR312
 00008 GOUT
 00009 MCODE4
 00010 MDATA1
 00011 MDATA1
 00012 MDATA1
 00013 MDATA1
 00014 MDATA1
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 00016 MDATA1
 00017 MDATA1
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 00019 MDATA1
 00020 MDATA1
 00021 MDATA1
 00022 MDATA1
 00023 MDATA1

STORAGE ASSIGNMENT (BLOCK, TYPE, RELATIVE LOCATION, NAME)

00001	000010	10L	0001	000260	100L	0001	000343	106L	0001	000405	110L	0001	000470	120L
00002	000022	130L	0001	000556	140L	0001	000574	150L	0001	000615	160L	0001	000633	170L
00003	000032	1726	0001	000037	1766	0001	000654	200L	0001	000107	2256	0001	000116	2326
00004	000070	300L	0001	000275	3066	0001	001003	310L	0001	000334	3276	0001	001033	330L
00005	001061	340L	0001	000424	3506	0001	001100	350L	0001	001115	360L	0001	000452	3616
00006	001134	370L	0001	001152	400L	0001	000667	4336	0001	000670	4366	0001	000741	4446
00007	000766	4756	0001	000060	50L	0001	001170	5516	0001	001175	5556	0001	000140	70L
00008	000722	800F	0000	000723	801F	0000	000736	802F	0000	000752	803F	0001	000221	90L
00009	000555	95L	0000	000113	AMUM	0000	000360	0FNS	0000	000264	ENTH	0000	000571	EXMPIA
00010	000604	EXMPIB	0000	000614	EXMPI2	0000	000622	EXMPI2B	0000	000627	EXMPI3	0000	000634	EXMPI3B
00011	000643	EXMPI4	0000	000647	EXMPI5	0000	000653	EXMPI6	0000	000660	EXMPI7	0000	000303	FAZ
00012	000341	FOA	0000	000715	I	0000	000721	ICHNG	0000	000712	IDUM	0000	001006	INJPI
00013	000113	IO	0000	000717	IOPI	0000	000467	IOPI	0000	000664	IREAL1	0000	000716	J
00014	000702	L2MCD	0000	000377	LINE1	0000	000424	LINE2	0000	000447	LINE3	0000	000514	MOU14
00015	000531	MCODE4	0000	000245	MOLLE	0000	000720	N	0000	000000	NAME	0000	000714	NPLAC
00016	000220	PICT	0000	000670	WUM	0003	000000	WYES	0000	000322	WTEMP			

COMPUTING RELATIVE FIRST
 CENTRAL FIRST, WYES

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[illegible]

C-64

133.1	IF ICHNG-LE-1 .OR. ICHNG-GE-7) GO TO 106	000352
133.3	GO TO 110,120,130,140,150,160,170), ICHNG	000370
134	CONTINUE	000405
134.1	110	000406
134.2	CALL GOUTIEAMP1A,66)	000413
134.3	CALL GOUTIEAMP1B,48)	000424
134.4	DO 112 1-1.5	000429
134.5	J=1-1.5*1	000431
134.6	FLO(0,36,RODUM(J))=FLO(0,36,NAME(N,1))	000434
134.7	RODUM(J,1)=ANUM(N,1)	000440
134.8	CONTINUE	000443
134.9	112	000452
135	CALL RDATAF(10,RODUM,5110)	000452
135.1	DO 114 1-1.5	000452
135.2	J=1-1.5*1	000460
135.3	FLO(0,36,NAME(N,1))=FLO(0,36,RODUM(J))	000460
135.4	CALL CHECKINAML(N,1)	000462
135.5	ANUM(N,1)=RODUM(J,1)	000466
135.6	CONTINUE	000466
135.7	114	000470
135.8	GO TO 100	000470
135.9	120	000500
136	CONTINUE	000507
136.1	CALL DMWRTF(EMP2,36,PECHT(N),6)	000511
136.2	CALL RDATAF(1,PECHT(N),5120)	000515
136.3	MULL(N)=1H	000520
136.4	IF (.NOT. (YESIEEMP2B,30)) GO TO 100	000520
136.5	MULL(N)=1HM	000522
136.6	GO TO 100	000522
136.7	130	000532
136.8	CONTINUE	000541
136.9	CALL DMWRTF(EMP3,30,ENTH(N),5)	000544
137	CALL RDATAF(1,ENTH(N),5130)	000554
137.1	NAML(N,5)=2H	000554
137.2	IF (YESIEEMP3B,42)) NAME(N,5)=2H00	000556
137.3	GO TO 100	000556
137.4	140	000562
137.5	CONTINUE	000572
137.6	CALL GOUTIEAMP4,24)	000572
137.7	CALL RCHAR(FAZ(N),1,1,5140)	000574
137.8	GO TO 100	000604
137.9	150	000613
138	CONTINUE	000613
138.1	CALL DMWRTF(EMP5,24,RTEMP(N),5150)	000615
138.2	CALL RDATAF(1,RTEMP(N),5150)	000615
138.3	GO TO 100	000621
138.4	160	000631
138.5	CONTINUE	000631
138.6	CALL GOUTIEAMP6,30)	000633
138.7	CALL RCHAR(FOX(N),1,1,5160)	000633
138.8	GO TO 100	000633
138.9	170	000633
139	CONTINUE	000633
139.1	CALL DMWRTF(EMP7,24,ODENS(N),5)	000633
139.2	CALL RDATAF(1,ODENS(N),5170)	000643
139.3	GO TO 100	000657
139.4	180	000657
139.5	DELETE A FACTANT	000657
139.6	CONTINUE	000659
139.7	190	
139.8	200	

639.51	1729	NHEAC=NREAC-1	000654
639.52	1730	DO 220 I=N,NREAC	000655
639.53	1731	DO 210 J=1,5	000656
639.54	1732	NAME(I,J)=NAME(I+1,J)	000657
639.55	1733	ANUM(I,J)=ANUM(I+1,J)	000658
639.56	1734	CONTINUE	000659
639.57	1735	PLCWT(I)=PLCWT(I+1)	000660
639.58	1736	MOL(I)=MOL(I+1)	000661
639.59	1737	ENTH(I)=ENTH(I+1)	000662
639.60	1738	FAZ(I)=FAZ(I+1)	000663
639.61	1739	TEMP(I)=TEMP(I+1)	000664
639.62	1740	FOXT(I)=FOXT(I+1)	000665
639.63	1741	DENS(I)=DENS(I+1)	000666
639.64	1742	CONTINUE	000667
639.65	1743	GO TO 50	000668
639.66	1744		000669
639.67	1745	ADD A REACTANT	000670
639.68	1746	CONTINUE	000671
639.69	1747	NHEAC=NREAC+1	000672
639.70	1748	N=NHEAC	000673
639.71	1749	CALL GOUTEXMP1A,66)	000674
639.72	1750	CALL GOUTEXMP1B,48)	000675
639.73	1751	DO 305 I=1,5	000676
639.74	1752	J=I-1)*2+1	000677
639.75	1753	ROOM(J)=2H	000678
639.76	1754	CONTINUE	000679
639.77	1755	CALL RDATAF110,ROOM,5300)	000680
639.78	1756	J=I-1)*2+1	000681
639.79	1757	FLOIO,36,NAME(N,I))=FLOIO,36,ROOM(J))	000682
639.80	1758	CALL CHECKNAME(N,I)	000683
639.81	1759	ANUM(N,I)=ROOM(J+1)	000684
639.82	1760	CONTINUE	000685
639.83	1761	CONTINUE	000686
639.84	1762	CALL GOUTEXMP2,36)	000687
639.85	1763	PLCWT(N)=0.	000688
639.86	1764	CALL RDATAF11,PLCWT(N),5310)	000689
639.87	1765	CONTINUE	000690
639.88	1766	MOL(N)=1H	000691
639.89	1767	IF (MOYE SLEXP2B,30)) MOLE(N)=1H	000692
639.90	1768	CONTINUE	000693
639.91	1769	CALL GOUTEXMP3,30)	000694
639.92	1770	ENTH(N)=0.	000695
639.93	1771	CALL RDATAF11,ENTH(N),5330)	000696
639.94	1772	IF (MOYE SLEXP3B,42)) NAME(N,5)=2H00	000697
639.95	1773	CONTINUE	000698
639.96	1774	CALL GOUTEXMP4,24)	000699
639.97	1775	FAZ(N)=1H5	000700
639.98	1776	CALL RDATAF12(N),1,-1,5340)	000701
639.99	1777	CONTINUE	000702
640.00	1778	CALL GOUTEXMP5,24)	000703
640.01	1779	TEMP(N)=0.	000704
640.02	1780	CALL RDATAF11,TEMP(N),5350)	000705
640.03	1781	CONTINUE	000706
640.04	1782	CALL GOUTEXMP6,30)	000707
640.05	1783		000708
640.06	1784		000709
640.07	1785		000710
640.08	1786		000711
640.09	1787		000712
640.10	1788		000713
640.11	1789		000714
640.12	1790		000715
640.13	1791		000716
640.14	1792		000717
640.15	1793		000718
640.16	1794		000719
640.17	1795		000720
640.18	1796		000721
640.19	1797		000722
640.20	1798		000723
640.21	1799		000724
640.22	1800		000725
640.23	1801		000726
640.24	1802		000727
640.25	1803		000728
640.26	1804		000729
640.27	1805		000730
640.28	1806		000731
640.29	1807		000732
640.30	1808		000733
640.31	1809		000734
640.32	1810		000735
640.33	1811		000736

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FOX(N)=1HF
CALL HCHAR(FOX(N),1,-1,$360)
CONTINUE
CALL GOUT(AMF7,24)
DENSIN=0.
CALL HDATAF(1,DENS(N),$370)
GO TO 50

STORE CASE TO FILE #
CONTINUE
REWIND IO
WRITE(10,B00) NREAC
DO 410 I=1,NREAC
  WRITE(10,B01) (NAME(I),J,ANUM(I,J),J=1,5),PECMT(I),MOLE(I),
  1 ENT(I),FAZ(I),WTEMP(I),FOX(I),DENS(I)
CONTINUE
WRITE(10,B03) IDUM
WRITE(10,B03) IDUM
ENDFILE IO
RETURN
FORMAT(13)
FORMAT(2X,5A2,F8.4,2X),/,F10.6,2X,A1,F13.4,4X,A1,F12.3,
  1 3X,A1,F12.5,1A1
FORMAT(1X,12,2X,5A2,F8.4,2X),F10.6,2X,A1,F13.4,4X,A1,F12.3,
  1 3X,A1,F12.5,1X)
FORMAT(A1)
END

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00134 2290
00135 2290
00136 2300
00137 2310
00140 2320
00141 2330
00142 2340
00144 2350
00144 2360
00145 2370
00144 2380
00145 2390
00150 2400
00153 2410
00153 2420
00171 2430
00173 2440
00176 2450
00191 2460
00192 2470
00193 2480
00194 2490
00194 2500
00195 2510
00195 2520
00196 2530
00197 2540
END FOX

SUBROUTINE SAVE ENTRY POINT 000463
 4LEOF ENTRY POINT 000466

STORAGE USED: CODE(1) 000471; DATA(1) 000065; BLANK COMMON(2) 000000

COMMON BLOCKS:

0003 CONSTS 000006
 0004 MOLLON 000010
 0005 SPECS 012120
 0006 MISC 001264
 0007 I60X 000091
 0010 ECC 000003

LATE-1AL REFERENCES (BLOCK, NAME)

0011 ACALC
 0012 EXP
 0013 NADUA
 0014 P1043
 0015 P1015
 0016 NERH34

STORAGE ASSIGNMENT (BLOCK, TYPE, RELATIVE LOCATION, NAME)

0001	000137	100L	0001	000056	13L	0001	000042	131G	0001	000073	15L	0001	000112	20L
0001	000161	200G	0001	000172	200L	0001	000207	207G	0001	000310	236G	0001	000417	303G
0001	000177	50L	0000	000013	730F	0001	000273	744L	0001	000304	745L	0001	000340	750L
0001	000347	760L	0000	000016	770F	0000	000026	780F	0000	000031	785F	0005	006034	A
0000	000570	AM	0006	00624	AM1	0006	000741	AMUM	0003	000000	ATMN	0006	000004	ATOM
0006	R 000504	ED	0006	R 000521	ROP	0007	L 000036	CALCH	0005	000000	COEF	0007	000001	CONVG
0006	000625	CPH1	0006	000564	CPSUM	0006	000604	DATA	0005	005670	DELM	0010	000002	DEMAND
0006	001167	DELS	0006	R 001261	ENML	0004	000000	END	0005	R 005360	ENLN	0006	R 001263	ENLSAV
0006	R 000000	ENM	0006	R 001262	ENSAVE	0006	R 001262	FF	0000	001073	ENTH	0006	R 000566	EGPAT
0006	001112	FAZ	0000	R 000003	FCAL	0000	R 000012	FF	0000	R 000002	FHM	0006	001150	FOX
0000	R 000001	F00	0004	000001	GAS	0003	000001	GNET	0010	000000	GRAPH	0007	000003	HP
0016	R 000572	MPP	0000	R 000011	MS	0006	R 000567	MSURU	0005	005524	HO	0007	I 000030	IC
0007	000000	IOERUG	0004	I 000002	IE	0007	000015	IMAT	0000	000040	INJPS	0007	L 000023	IONIS
0007	000021	IP	0007	I 000037	IGSAVE	0007	I 000016	IOI	0007	I 000005	ISV	0007	000034	IT
0005	I 011444	IUSE	0004	000003	IZERU	0000	I 000005	J	0007	I 000026	JLIQ	0010	I 000001	JOUT
0007	I 000025	J50L	0007	000031	J51	0007	000014	KMAT	0004	I 000009	LANK	0006	I 000463	LLMT
0007	000004	LL1	0007	I 000040	LSAVE	0004	000005	MOL	0007	I 000006	MOLES	0006	000426	NAME
0007	000004	NC	0007	000022	NEWB	0007	000035	NF2	0007	I 000012	NLM	0007	000017	NOF
0007	000020	NGMTT	0007	000007	NP	0007	I 000011	NPT	0007	000027	NPEAC	0006	000013	N5
0007	I 000000	N5PP1	0007	000010	NT	0006	R 000565	OF	0004	000006	OX	0006	001227	OXF
0007	I 000002	PATM	0006	001054	FE CMT	0006	000563	PP	0003	R 000003	PRAR	0003	000004	RHP
0007	R 000574	PH	0006	R 001206	PHOP	0006	001207	RHW	0006	001131	RTEMP	0003	000005	RVR
0005	002570	S	0007	000033	SHOCK	0005	R 011754	SLN	0007	000004	SP	0005	010770	SDB
0007	R 000000	SUM	0006	000001	SUMN	0006	000003	SN	0005	011610	TEMP	0006	000547	THIGH


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10105 EN(J,NPT) = EXP(LN(EN(J)))
10106 50 CONTINUE
10107 NEM = LL1
10108 RETURN
10109
10110 C FIRST T-SAVE COMPOSITIONS FOR FUTURE POINTS WITH (HIS T
10111 100 ISV = -15V
10112 ICSAVE = ICI
10113 ENSAVE = ENN
10114 ENLSAV = ENNL
10115 LSAVE = LLMT(NLM)
10116 N0 150 J = 1,N5
10117 EN(J,NPT) = EN(J,ISV)
10118 EN(J) = ENL(NJ)
10119 IF (IUSE(IJ) .NE. 0) SLN(J) = EN(J,ISV)
10120 C USE COMPOSITIONS FROM PREVIOUS POINT
10121 200 DO 300 J = 1,N5
10122 EN(J,NPT) = EN(J,ISV)
10123 RETURN
10124
10125 C CALCULATE NEW VALUES OF BD AND HSUBU FOR NEW OF RATIO
10126 ENTRY NEWOF
10127 WRITE(JOUT,730) OF
10128 730 FORMAT(6HOF = ,F10.6)
10129 SUM = 0F + 1.
10130 V2 = (OF*VMIN(1)+VMIN(2))/SUM
10131 V1 = (OF*VPLS(1)+VPLS(2))/SUM
10132 IF (V2 .LT. 0.0) EQRT = ABS(V1/V2)
10133 IF (RH(1) .GT. 0.0 .AND. RH(2) .GT. 0.0) GO TO 744
10134 RHOP = RH(2)
10135 IF (RHOP .LE. 0.0) RHOP = RH(1)
10136 GO TO 745
10137
10138 744 RHOP = (OF*1.0+RH(1)+RH(2))/(RH(1)+ OF *RH(2))
10139 745 DO 747 J = 1,NLM
10140 747 BD(J) = (BUP(J,2) + BOP(J,1)*OF)/SUM
10141 NPT = 1
10142 IF (.NOT.CALCH) GO TO 750
10143 CALL HCALL
10144 CALCH = .FALSE.
10145 IF (OF .GT. 0.0) HPP(1) = SUM*HPP(1)/OF
10146 HPP(2) = SUM*HPP(2)
10147 DO 760 J = 1,NLM
10148 750 HSUBU = (HPP(2) + HPP(1)*OF)/(ERRAR*SUM)
10149 760 IC = 0
10150 JSOL = 0
10151 JULU = 0
10152 H5 = R6AR*H5SUBU
10153 WRITE(JOUT,773)
10154 773 FORMAT (14U,17X,4HFUEL ,13X,7HOXIDANT ,12X,7HMIXTURE //)
10155 780 FORMAT (14 ,5L18.8/)
10156 FF = FHH
10157 IF (VULIFF = FUU)
10158 WRITE(JOUT,780) FF,FCAL ,HPP(2),HPP(1),H5
10159 785 FORMAT (12H KG-ATOMS/KG)
10160 785 FORMAT (12H KG-ATOMS/KG)
10161 WRITE(JOUT,780) (LLMT(IJ),LANH,BOP(J,2),BUP(J,1),BD(J), J = 1,NLM)
10162 RETURN
10163 END

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MAIN0139

MAIN0124
MAIN012

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000005 UL-15-SLAMCHOUTS-SEARCH
000001 13-10/25/79-17:40:07 (9.1)

SUBROUTINE SEARCH ENTRY POINT 000024

STORAGE USED: CODE(1) 000000; DATA(1) 000114; BLANK COMMON(2) 000000

COMMON BLOCKS:

00003 HOLCON 000010
00004 SPECS 012120
00005 MISC 001264
00006 INDX 000041
00007 CCC 000003

LABEL REFERENCE (BLOCK, NAME)

00010 NAME
00011 NAME
00012 NAME
00013 NAME
00014 NAME

STORAGE ASSIGNMENT (BLOCK, TYPE, RELATIVE LOCATION, NAME)

00000	000022	10F	00001	000014	1236	00001	000015	1266
00001	000075	1526	0001	000120	1676	0001	000306	170L
00002	000045	172F	0000	000055	176F	0000	000030	20F
00003	000177	2166	0001	000204	2236	0001	000215	2316
00004	000371	3046	0000	000020	5F	0001	000035	7L
00005	000220	420L	0001	000227	825L	0000	000032	871F
00006	000624	AM	0005	000741	ANUM	0005	000004	ATOM
00007	000521	60P	0006	000036	CALCH	0004	000000	COEF
00008	000564	CP5UM	0005	000604	DATA	0004	R 002734	DATE
00009	001167	DLNS	0004	002734	EN	0003	I 000000	END
00010	000000	LNN	0005	001261	LNNL	0005	001262	LSAVE
00011	001112	FAZ	0005	001150	FOX	0003	I 000001	GAS
00012	000572	HPP	0005	000567	MSUBU	0004	005524	MO
00013	000000	ICERUB	0003	000002	IE	0006	000015	IMAT
00014	000021	IP	0006	000037	IOSAVE	0006	000016	IOI
00015	I 011444	IOSE	0000	I 000012	IX	0003	000003	I2EPO
00016	I 000001	JOUT	0006	000025	J50L	0006	000031	J51
00017	I 000012	L	0003	000004	LANK	0005	I 000463	LLMT
00018	000006	MOLES	0000	I 000005	MT	0005	000626	NAME
00019	000035	NF2	0006	000017	Nof	0006	I 000020	NOM11
00020	000027	NRLAC	0006	I 000013	N5	0000	I 000000	NSPFI
00021	I 005360	OMIT	0003	000006	OK	0005	001227	OKF
00022	000563	PF	0005	000574	KH	0005	001206	QHOP
00023	002570	S	0006	000033	SHOCK	0004	011754	SUN
00024	I 000001	SOME	0006	000003	SO	0004	R 011610	TEMP
00025	000560	TLO	0005	000557	TM	0005	R 000561	THIO
00026	000015	TI	0006	000016	T2	0005	000576	VMIN

0001	000043	1446	0001	000013	I	0000	I 000003	IC
0001	000121	1716	0001	000066	INJPS	0006	000023	ION5
0001	000137	2026	0006	000005	ISV	0006	000034	IT
0001	000271	2526	0000	000014	J	0006	000026	JL10
0001	000164	410L	0000	I 000017	K	0006	000014	PMAT
0005	000570	AM	0006	000040	LSAVE	0003	000005	MOL
0005	000502	BN	0006	I 000024	NC	0006	000022	NCLP
0005	000625	CPPI	0006	000007	NP	0006	000011	NFT
0007	000002	DEMAND	0005	000010	NT	0005	000565	OF
0005	001263	ENLSAV	0000	001054	PECM1	0000	I 000011	PHAT
0005	000566	EGPAT	0005	001207	PHM	0005	001131	PLE4P
0006	000003	HP	0006	000004	SP	0004	I 010770	SOP
0006	000030	IC	0005	R 000562	TIGH	0005	001226	TLN
0006	000023	ION5	0006	000002	TP	0006	000002	TT
0006	000034	IT	0006	000032	VOL	0006	000600	VFL5

4005 000602 MP

0003 000007 ZERO

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1001 SUBROUTINE SEARCH
1002 C SEARCH TAPE FOR THERMO DATA FOR SPECIES TO BE CONSIDERED
1003 C
1004 C
1005 COMMON /HOLCON/ END,GAS,IE,IZERO,LANK,MOL,OX,ZERO
1006 COMMON/SPECES/COEF(2,7,150),S(150),EN(150,3),ENL(150),HOL(150)
1007 C 1 DELN(150),AL(15,150),SUB(150,3),JUSE(150),TEMP(50,2),SLN(150)
1008 C INCLUDE SPECPR
1009 C
1010 COMMON /MISC/ ENN,SUMN,TI,SO,ATOM(3,101),LLMT(15),BO(15),
1011 BUP(15,2),IM,TLOW,IMID,TMIGH,PP,CPSUM,OF,EQRAT,
1012 HSUBD,AM(2),HPP(2),RMT(2),VMIN(2),VPLS(2),NP(2),
1013 DATA(16),AM1,CPRI,NAME(15,5),ANUM(15,5),PECT(15),
1014 ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15),RHOP,
1015 RMW(15),TLN,USF(26),ENNL,ENSAVE,ENLSAV
1016 C
1017 COMMON /INDX/ IDBUG,CONVG,TP,MP,SP,ISV,MOLES,NP,MT,NPI,L,NS,
1018 KMAT,IMAT,IOI,NOF,NOMIT,IP,NEWIR,IOMS,NC,JSL,JLIQ,
1019 NREAC,IC,JSI,VOL,SHOCK,IT,NFZ,CALCH,IOSAVE,LSAVE
1020 C
1021 C
1022 COMMON /CCC/ GRAPH,JOUT,DEMAND
1023 C
1024 C
1025 DIMENSION B(4),DATE(2,3),MT(4),OMIT(3,3)
1026 EQUIVALENCE (DATE,ENT),IENLN,OMIT)
1027 INTEGER END,GAS,OMIT,PHAZ,SUB
1028 LOGICAL NEW
1029 C
1030 NC=0
1031 IX=0
1032 SUB(1,1)=END
1033 DO 3 I=1,150
1034 DO 3 J=1,L
1035 3 A(I,J)=0.0
1036 READ(4,5) TLOW,IMID,TMIGH
1037 5 FORMAT (3F10.3)
1038 NS=1
1039 7 READ (4,10)(SUB(INS,I),I=1,3),DATE(1,NS),DATE(2,NS),(MT(I),B(I),
1040 I=1,4),PHAZ,11,12
1041 10 FORMAT(3A4,6X,2A3,4I42,F3.0),A1,2F10.3)
1042 IF (SUB(INS,1).EQ.END) GO TO 171
1043 HEAD (4,20) ((COEF(I),J,NS),J=1,7),I=1,2)
1044 20 FORMAT (5E15.8)
1045 IF (NGMIT.EQ.0) GO TO 810
1046 DO BUS I=1,NOMIT
1047 DO BUS J=1,3
1048 GO TO 7
1049 804 IF (OMIT(J,1).NE. SUB(INS,J)) GO TO BUS
1050 GO TO 7
1051 BUS CONTINUE
1052 DO 40 K=1,4
1053 IF (B(K).EQ.0.) GO TO 825
1054 DO 16F I=1,L
1055 IF (ALLT(I).EQ. MT(K)) GO TO 820
1056 GO 519 J=1,L
1057 519
1058 519
1059 519
1060 519
1061 519
1062 0

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/HOLCON/

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819 A(I,J,NS) = 0.
   GO TO 7
820 A(I,NS) = B(K)
825 IUSE(NS) = 0
   IF (FHAZ-EG.GAS) GO TO 170
   NC = NC+1
   TEMPINC(1) = 11
   TEMPINC(2) = 12
   IX = IX+1
   IF (IUSE(NS)-1).EQ.0 .OR. NC.EQ.1) GO TO 145
   DO 830 I=1,L
830 IF (A(I,NS) .NE. A(I,NS-1)) GO TO 145
   IX = IX+1
145 IUSE(NS) = -IX
170 NS = NS+1
   IF (NS .LT. NSPP1) GO TO 7
   WRITE (JOUT,R71)
871 FORMAT (//20X,54HDIMENSIONS IN /SPECIES/ FOUND TO BE TOO SMALL IN S
      ILARCH/)
171 NS = NS-1
   NEWRE = .FALSE.
   WRITE (JOUT,I72)
172 FORMAT(42H0SPECIES BEING CONSIDERED IN THIS SYSTEM )
   DO 174 I=1,NS,5
     K = 1 + 4
     IF (NS .LT. K) K = NS
174 WRITE (JOUT,I76) DATE(1,J), DATE(2,J), SUB(J,1), SUB(J,2), SUB(J,3),
       1 J=1,M
176 FORMAT(51X,24J,2X,3AN)
   RETURN
   END

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000251
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000260
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000264
000266
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000270
000271
000273
000274
000277
000300
000402
000402
000415
000416
000417
END FOR

OF ON 5 LE 15-SHCH-LE 15-SHCH
 ***A ** -10/25/77-17:40:16 (10.1)

SUBROUTINE SHCH ENTRY POINT 001367

STORAGE USED: CODE(1) 001401; DATA(0) 000263; BLANK COMMON(2) 000000

COMMON BLOCKS:

0003 CONSTS 000006
 0004 HOLCON 000010
 0005 POINTS 000335
 0006 SPECS 01.120
 0007 PTSC 001264
 0010 DOUBLE 001560
 0011 INDX 000041
 0012 PLRF 000166
 0013 OUPF 000073
 0014 CCC 000003

EXTERNAL REFERENCES (BLOCK, NAME)

0015 KUYLS
 0016 PAGIT
 0017 CHS14
 0018 GOUT
 0019 PLWOF
 0020 MCALC
 0021 GUT1
 0022 GUT2
 0023 LCLDEM
 0024 SAVE
 0025 GUT3
 0026 N-ML3
 0027 N-ML3
 0028 N-ML3
 0029 N-ML3
 0030 N-ML3
 0031 N-ML3
 0032 N-ML3
 0033 N-ML3
 0034 N-ML3
 0035 N-ML3
 0036 N-ML3
 0037 ALUG
 0040 EXP
 0041 NLRM34

STORAGE ASSIGNMENT (BLOCK, TYPE, RELATIVE LOCATION, NAME)

0000	CODE	000143	125F	0001	000211	14L	0001	000111	1456	0001	000221	15L	0001	001001	150L
0001	CODE	000163	152F	0001	000124	1566	0001	000101	16F	0001	001112	161L	0001	000126	17L
0002	CODE	000143	19L	0001	000073	2046	0001	000114	21L	0001	000136	2236	0001	000147	2316
0003	CODE	000143	30L	0001	000356	3236	0001	000376	3346	0001	000520	3616	0001	000534	40L
0004	CODE	001123	411L	0001	000320	44L	0001	000325	45L	0001	000137	46F	0001	001057	4616
0005	CODE	000143	47L	0001	000547	51L	0001	001201	5206	0001	001232	5366	0001	001247	5476

[illegible]

VP(13)
C(13), VP(13)
SD, HO(150)
I, SLN(150)

COMMON /CONSIST/ ATTN, GMEI, P, IM, D, BAW, WBR, D, VR

COMMON /CONS/ ALPH.GMEL.PAIN.DBAH.WBR.DVR

COMMON /HOLCON/ LNU,6A5,IL,1ZERO,LANK,MOL,0X,ZERO

COMMON/POINTS/MSUM(I3),SSUM(I3),CPH(I3),ULVPI(I3),DLVPI(I3)

• GARMASIS, P (201).

,0120(13),09N(13)
000000SPRINTS/COF F(2,7,150),SPRINTS(150),HDI(150)

0.015, 150), 506 (150, 3), 1056 (150), 1666 (50, 2), 1696 (150)

THE

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10112 COMMON /MISC/ LNN,SUMN,TT,SD,ATOM13,101,LLMT151,B01151,
10113 B0P115,27,IM,TLOW,IMID,THIGH,PP,CPSUM,OF,EQRAT,
10114 HSUBU,AM121,HP121,RH121,VH121,VPL121,WP121,
10115 UATA116,AM1,CP1,NAME115,51,ANUM115,51,PECM1151,
10116 LETH1151,FA21151,RTMP1151,FOX1151,DENS1151,RHOP,
10117 LM1151,TLN,OXF1261,ENML,ENSAVE,ENLSAV
10118 COMMON /DOUPLE/ G120,211, X1201
10119 COMMON /INDX/ IOLRUG,CONVG,TP,HP,SP,ISV,MOLES,NP,NT,NPT,MLM,NS,
10120 AMAT,IMAT,IQ1,NOF,NOMIT,IP,NEUR,IONS,NC,JSOL,JL1Q,
10121 NOLAC,IC,JS1,VOL,SHOCK,IT,NF2,CALCH,IOSAVE,LSAVE
10122 COMMON /PERF/ PCP1261,VMOC1131,T211111,UIU21131,UI1131,
10123 NACH1113,RRH01131,M2M1131,EQL
10124 COMMON /OUP1/ F9X,F13,FA,FAP121,FR,FC,FCP131,FCST121,FCV,FG121,
10125 FGL,FGV,FH121,F1121,F1121,FM121,FM1151,FN121,FOUR,
10126 FP,F5121,FSV,FT121,FT121,FV121,FVEL121,ONE,THREE,
10127 TWO,ELROF
10128 COMMON /CCC/ GRAPH,JOUT,DEMAND
10129
10130 DATA FMM/6M2/M1 /,FPP/6M2/P1 /,FPA/6M2/H02/P1,FRB/6M2/H01 /,
10131 F11/6M2/P1 /,FUI/6M2/H01 VE/,FU2/6M2 VE/,FV21/6M2/H01-1,
10132 FV22/6M2/H01/S/,FV23/2HEC/
10133 DOUBLE PRECISION G,G6,X
10134 EQUIVALENCE IX1N1,G61
10135 LOGICAL EQL,INDEU,INCOF2,SEUL,TP
10136
10137 LOGICAL ROYLS
10138
10139 REAL M1,MACH1,M2M1,MUI2PT
10140 NAMELIST /SHRIMP/ GAMMA1,INCOF6,INCOF7,MACH1,UI
10141
10142 IF = 0
10143 IF = .TRUE.
10144 CP1 = 0.
10145 UO 10 1 = 1.13
10146 MACH111 = 0.
10147 UI111 = 0.0
10148 GAMMA1 = 0.
10149 INCOF6 = .TRUE.
10150 INCOF7 = .TRUE.
10151 UO 10 1 = 1,NLAC
10152 NAME11,51 = 12,RO
10153 CALL PAG11
10154 CALL CHRS17111
10155 IF INDI111,TYPEL YES FOR PRESENT VALUES OF SHRIMP NAMELIST*,4611
10156
10157 1 WRITE(6,SHRIMP)
10158 CALL CHRS17111
10159 READ 15,SHRIMP)
10160 WRITE(JOUT,SHRIMP)
10161 SEUL = INCOF6
10162 IF (UI111) .LE. 0.01 T111 = R111111
10163 UO 10 1 = 1.17
10164 IF (MACH111) .LE. 0.0 .AND. UI111 .LE. 0.01 GO TO 71
10165
10166 IF 150 = 1

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00343 1230
00344 1240
00345 1250
00346 1260
00347 1270
00348 1280
00349 1290
00350 1300
00351 1310
00352 1320
00353 1330
00354 1340
00355 1350
00356 1360
00357 1370
00358 1380
00359 1390
00360 1400
00361 1410
00362 1420
00363 1430
00364 1440
00365 1450
00366 1460
00367 1470
00368 1480
00369 1490
00370 1500
00371 1510
00372 1520
00373 1530
00374 1540
00375 1550
00376 1560
00377 1570
00378 1580
00379 1590
00380 1600
00381 1610
00382 1620
00383 1630
00384 1640
00385 1650
00386 1660
00387 1670
00388 1680
00389 1690
00390 1700
00391 1710
00392 1720
00393 1730
00394 1740
00395 1750
00396 1760
00397 1770
00398 1780
00399 1790

NPT = 1
47 GAMMA1 = GAMMA5(NPT)
M1 = MM(NPT)
P1 = PP(NPT)
T1 = TT(NPT)
HS = HSUM(NPT)
P21 = (2.*GAMMA1*HACH1(NPT)**2-GAMMA1+1.)/(GAMMA1+1.)
T21 = P21*(2.*HACH1(NPT)**2+GAMMA1-1.)/(GAMMA1+1.)
IF (T1**1211-61-2000.-AND. EQL) T21 = .7*T21 + 600./T1
MUL2RT = AM1*U1(NPT)**2/(RBR**11)
P21L=ALOG(P21)
T21L=ALOG(T21)
DO 100 I = 1,R
  TT=T21**I
  PP=P21**I
  IF (.NOT.EQL) GO TO 40
  CALL EQLBRM
  GO TO 50
C
  FROZEN
  40 T1L = ALOG (T1)
  CALL HCALLC
  HSUM(NPT) = HSUBU
  CPR(NPT) = CPR1
  50 RH012 = M1*T21/(MM(NPT)*P21)
  GG=RH012*MUL2RT
  G(1,1)=GG*DLVFT(NPT)-P21
  G(1,2)=GG*DLVTP(NPT)
  G(1,3)=P21-1.+MUL2RT*(RH012-1.)
  GG = (U1(NPT)*RH012)**2/RBR
  G(2,1)=GG*DLVFT(NPT)+T1*DLVTP(NPT)-1.1/MM(NPT)
  G(2,2)=GG*DLVTP(NPT)-T1*CPR(NPT)
  G(2,3) = HSUM(NPT) - HS - U1(NPT)**2*(1.0 - RH012**2)/(2.0*RBR)
  X(1)=G(1,1)*G(2,2)-G(1,2)*G(2,1)
  X(1)=G(1,3)*G(2,2)-G(1,2)*G(2,3)+G(1,2)*X(3)
  X(2)=G(1,1)*G(2,3)-G(1,2)*G(2,1)*X(3)
  AX = X(1)
  AX = X(2)
  IF (AX*LT.0.) AX = -AX
  IF (AX*LT.0.) AX = -AX
  IF (AX*GT.0.) AX = AX
  IF (AX*LT.00005) GO TO 150
  AX = AX/.4054652
  IF (AX*LE.1.) GO TO 75
  X(1) = X(1)/AX
  X(2) = X(2)/AX
  75 P21L=P21L+X(1)
  T21L=T21L+X(2)
  P21=EXP(P21L)
  100 T21 = EXP(T21L)
  110 RTE(JOUT,125) U1(NPT)
  125 FORMAT(25H: DID NOT CONVERGE FOR U1=,FR.2,66H
  1T RELIABLE, SOLUTION PROBABLY DOES NOT EXIST)
  150 RH012NPT = 1./RH012
  H2M1(NPT) = H2CPR1/AM1
  PCPR(NPT) = P21
  T21(NPT) = T21
  ANSWERS PROBABLY NO
000407
000412
000414
000416
000420
000422
000424
000436
000453
000473
000503
000507
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000753
000757
000763
000771
001001
001001
001001
001004
001007
001013

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00495 1799 IF (NPT .GE. 100000 .AND. 100000 .NE. 0) WRITE(JOUT,152) I,121,P21
00496 1800 152 FORMAT(10HOUT NO.=,I1,7X,7H12/11 =,F9.2,7X,7HP2/P1 =,F9.2 )
00497 1801 UTWO(NPT) = UT(NPT)*RH012
00498 1802 U12(NPT) = U1(NPT)*UTWO(NPT)
00499 1803 IF (.NOT.EQL) GO TO 161
00500 1804 DO 880 K=1,N5
00501 1805 IF (IUSL(N),LT,0) GO TO 880
00502 1806 IF (ENL(N),GT,-87 .AND. ENL(N),LT,87.) EN(M,NPT) = EXP(ENL(N))
00503 1807 880 CONTINUE
00504 1808 GO TO 431
00505 1809 C FROZEN
00506 1810 161 PP(NPT) = PP
00507 1811 TT(NPT) = TT
00508 1812 GAMMA(NPT) = CPRINT/(CPR(NPT) - 1.0/AM1)
00509 1813 431 15V = 0
00510 1814 IF (NPT,LT,NSK) 15V=NPT
00511 1815 IF (NPT,GT,1) 15V=-1
00512 1816 NPT = NPT+1
00513 1817 IF (EQL) CALL SAVE
00514 1818 IF (NPT,LE,NSK) GO TO 47
00515 1819 NPT = NSK
00516 1820 C OUTPUT--2ND CONDITION
00517 1821 WRITE(JOUT,58)
00518 1822 58 FORMAT (16HSHOCKED GAS (2) )
00519 1823 FMT(4) = TWO
00520 1824 WRITE(JOUT,FMT) FU2,FVEL,(UTWO(J),J = 1,NPT)
00521 1825 CALL OUT2
00522 1826 WRITE(JOUT,68)
00523 1827 68 FORMAT (26HINCIDENT SHOCK PARAMETERS )
00524 1828 FMT(4) = THREE
00525 1829 WRITE(JOUT,FMT) FPP,FB,FB,(PCPJ),J = 1,NPT)
00526 1830 WRITE(JOUT,FMT) FTT,FB,FB,(T2T1(J),J = 1,NPT)
00527 1831 FMT(4) = FOUR
00528 1832 WRITE(JOUT,FMT) FMM,FB,FB,(M2M1(J),J = 1,NPT)
00529 1833 WRITE(JOUT,FMT) FRA,FB,FB,(RRHO(J),J = 1,NPT)
00530 1834 FMT(4) = TWO
00531 1835 WRITE(JOUT,FMT) FV21,FV22,FV23,(U12U2(J),J = 1,NPT)
00532 1836 CALL OUT3
00533 1837 INCULC = .FALSE.
00534 1838 IF (INCULC .AND. EQL) GO TO 17
00535 1839 IF (10F,LT,NOF) GO TO 21
00536 1840 TP = .FALSE.
00537 1841 DO 999 K = 1,NHEAC
00538 1842 999 RTMP(K) = T(1)
00539 1843 RETURN
00540 1844 END
00541 1845
00542 1846 FOR

```


FORM 5 LEWIS.THERMP.LEWIS.THERMP
H.A. 13-10/25/79-17:40:27 (B.)

SUBROUTINE THERMP ENTRY POINT 000376

STORAGE USED: C00111 000400; DATA01 00111; BLANK COMMON(2) 000000

COMMON BLOCKS:

C0005 CONSTS 000006
C0009 F01HIS 000335
C0005 MISC 001264
C0006 T40X 000091
C0007 00PT 000073
C0010 CCC 000003

EXTERNAL REFERENCES (BLOCK, NAME)

0011 HELWOF
0012 ECL6M
0013 C011
0014 C014
0015 C013
0016 SAVL
0017 N4005
0018 *10.3
0019 *10.3
0020 N4033

STO, AGE ASSIGNMENT (BLOCK, TYPE, RELATIVE LOCATION, NAME)

0000	000017 10F	0000	000023 11F	0000	000031 12F	0001	000022 1246	0001	000044 1316
0000	000037 20F	0000	000043 21F	0001	000220 2176	0001	000052 22F	0001	000245 2336
0000	000004 SF	0001	000061 800L	0001	000111 860L	0001	000146 861L	0001	000173 862L
0000	000060 863F	0001	000251 864L	0000	000066 868F	0001	000323 870L	0001	000352 871L
0001	000006 95L	0005	000570 AM	0005	000624 AM	0005	000741 ANUM	0003	000000 ATMH
0005	000004 ATOM	0005	000502 B0	0005	000521 BOP	0006	000036 CALCH	0006	000001 CONVG
0004	000032 CPH	0005	000625 CFRI	0005	000564 CPSUM	0010	000604 DATA	0010	000002 DEMAND
0005	001167 DLS	0004	000064 DLYPT	0004	000047 DLYTP	0005	001263 ENLSAV	0005	000000 ENN
0005	001261 ENML	0005	001262 ENSAVE	0005	001073 ENTH	0005	000566 EQRAI	0007	000002 FA
0007	000003 FAP	0005	001112 FAZ	0007	R 000005 FR	0007	000006 FC	0007	000007 FCP
0007	000012 FCST	0007	000014 FCV	0007	000015 FG	0007	000017 FGE	0007	000020 FGV
0007	000021 FH	0007	000023 FI	0007	000025 FIV	0007	000027 FM	0007	R 000031 FMT
0007	000050 FH	0007	000052 FOUR	0005	001150 FOX	0007	000053 FP	0007	R 000054 FS
0007	000056 FSV	0007	000057 FI	0007	000061 FIK	0000	000000 FUA	0000	R 000001 FUP
0007	000063 FV	0007	000065 FVEL	0007	000001 F13	0004	000000 F9A	0004	R 000101 GAMHAS
0007	000001 JMET	0010	000000 GRAPH	0006	L 000003 HP	0005	000572 HPP	0005	R 000567 HSUBU
0007	000000 HSUM	0000	000003 I	0006	000030 IC	0006	I 000000 IDEBUG	0006	R 000015 IMAT
0000	000072 INJP	0000	000002 IOF	0006	I 000023 IONS	0006	I 000021 IP	0006	R 000037 IOSAVE
0000	000016 JCI	0006	I 000005 ISV	0006	I 000034 IT	0006	000026 JLIQ	0010	I 000001 JOUT
0000	000025 J'HL	0006	J00031 J51	0006	000014 KHAT	0005	000043 LLMT	0006	R 000040 LSARE
0006	000006 KOLF	0005	000026 NAME	0006	000024 NC	0006	000022 NEWB	0006	R 000035 NFZ


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000104      ISV = NPT
000105      IF (NPT.NE.13) GO TO 870
000106      860 WRITE(JOUT,5)
000107      5 FORMAT(1H1,41X,48THERMODYNAMIC EQUILIBRIUM PROPERTIES AT ASSIGNED MOLI0032
000108      1)
000109      IF (.NOT.VOL) GO TO 861
000110      IF (NPT) WRITE(JOUT,10)
000111      10 FORMAT(1H0,62X,7H VOLUME /)
000112      IF (TPT) WRITE(JOUT,11)
000113      11 FORMAT(1H0,54X,22HTEMPERATURE AND VOLUME /)
000114      IF (SP) WRITE(JOUT,12)
000115      12 FORMAT(1H0,56X,18HENTROPY AND VOLUME /)
000116      GO TO 862
000117      861 IF (NPT) WRITE(JOUT,20)
000118      20 FORMAT(1H0,62X,10H PRESSURES /)
000119      IF (TP) WRITE(JOUT,21)
000120      21 FORMAT(1H0,53X,24HTEMPERATURE AND PRESSURE /)
000121      IF (SP) WRITE(JOUT,22)
000122      22 FORMAT(1H0,55X,20HENTROPY AND PRESSURE /)
000123      862 CALL OUT1
000124      WRITE(JOUT,863)
000125      863 FORMAT (25HOTHERMODYNAMIC PROPERTIES//)
000126      IF (.NOT.VOL) GO TO 864
000127      FMT(3) = ONE
000128      IF (.NOT.NPT) GO TO 864
000129      DO 63 I=1,NPT
000130      FMT(I*2) = TWO
000131      IF (I.EQ.13) FMT(15) = 5HF9.2)
000132      63 V(I) = RBAR*SUBU
000133      WRITE(JOUT,FMT) FUA,FUB,FB,(V(I), I = 1,NPT)
000134      864 CALL OUT2
000135      CALL OUT3
000136      IF (ISV.EQ.0 .AND. IOF.EQ.NOF) RETURN
000137      IF (IOFUG.GT.13) IOFUG=IOFUG-13
000138      WRITE(JOUT,868)
000139      868 FORMAT(1H1)
000140      IF (INT*LG.1.AND.NP.EG.1) GO TO 95
000141      NPT = 0
000142      870 NPT = NPT + 1
000143      IF (.NOT.TP) T(1)=IT
000144      IF (IF*LG.1.AND.II.EG.1) ISV=-ISV
000145      IF (INT*LG.1) GO TO 871
000146      IF (IT.EG.NT) ISV=0
000147      871 CALL SAVE
000148      GO TO 95
000149      END

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MOLI0037

12-22

12-22

MOLI0045

C-83

000071
000102
000102
000123

IF (V11) .GE. 1.0E6) FMT(15) = FZERO
45 CONTINUE
RETURN
END

00141 240
00143 250
00145 260
00146 270
END FOR

-SCRIPT PRINTS

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